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         FEB 16
                 STN Express Maintenance Release, Version 8.4.2, Is
                 Now Available for Download
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         FEB 16
                 Derwent World Patents Index (DWPI) Revises Indexing
                 of Author Abstracts
                 New FASTA Display Formats Added to USGENE and PCTGEN
NEWS
      6 FEB 16
NEWS
     7 FEB 16
                 INPADOCDB and INPAFAMDB Enriched with New Content
                 and Features
NEWS 8 FEB 16
                 INSPEC Adding Its Own IPC codes and Author's E-mail
                 Addresses
         APR 02
NEWS 9
                 CAS Registry Number Crossover Limits Increased to
                 500,000 in Key STN Databases
NEWS 10
         APR 02
                 PATDPAFULL: Application and priority number formats
                 enhanced
NEWS 11
         APR 02
                 DWPI: New display format ALLSTR available
NEWS 12
         APR 02
                 New Thesaurus Added to Derwent Databases for Smooth
                 Sailing through U.S. Patent Codes
NEWS 13
         APR 02
                 EMBASE Adds Unique Records from MEDLINE, Expanding
                 Coverage back to 1948
                 CA/CAplus CLASS Display Streamlined with Removal of
NEWS 14
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                 Pre-IPC 8 Data Fields
NEWS 15
         APR 07
                 50,000 World Traditional Medicine (WTM) Patents Now
                 Available in CAplus
NEWS 16 APR 07 MEDLINE Coverage Is Extended Back to 1947
NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
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AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

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TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

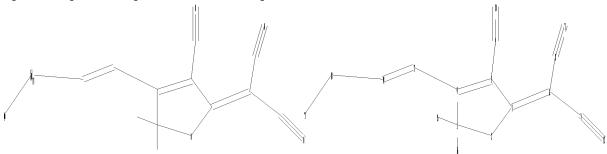
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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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chain nodes :
6 7 8 9 17 18
ring nodes :
1 2 3 4 5
ring/chain nodes :
10 11 12 13 14 15 16
chain bonds :
1-6 3-15 3-16 4-13 5-9 6-7 6-8 7-12 8-11 9-10 14-18 17-18

ring/chain bonds :

13 - 14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 7-12 \quad 8-11 \quad 9-10 \quad 13-14 \quad 14-18 \quad 17-18$ 

exact bonds :

1-6 3-15 3-16 4-13 5-9 6-7 6-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

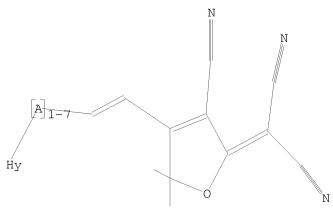
18:CLASS

### L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 14:57:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 59 TO ITERATE

100.0% PROCESSED 59 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 720 TO 1640 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 14:57:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1014 TO ITERATE

100.0% PROCESSED 1014 ITERATIONS SEARCH TIME: 00.00.01

14 ANSWERS

L3 14 SEA SSS FUL L1

=> d scan

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[4-[4-[5-[2-[4-[bis(2-

mercaptoethyl)amino]phenyl]ethenyl]-3,-dihexyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]-, polymer with
1,1'-(2,2',3,3',5,5',6,6'-octafluoro[1,1'-biphenyl]-4,4'-diyl)bis[1H-pyrrole-2,5-dione] and 4,4'-thiobis[benzenethiol]
MF (C47 H52 C12 N4 O S3 . C20 H4 F8 N2 O4 . C12 H10 S3)x
CI FMS

CM 1

PAGE 1-A

PAGE 2-A

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[4-(1-pyrrolidinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]- C18 H18 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):111

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]-MF C51 H60 N4 O3 S

Double bond geometry as shown.

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2 (3-eyano-5-(3, 4-dichlorophenyl)-4-[(1E,3E)-4-[5-[(1E)-2-(4-(dichylamino)phenyl]ethenyl]-3, 4-dihexyl-2-thienyl]-1,3-butadien-1-yl-5-methyl-2(5B)-furanylidene]MF C47 H52 C12 N4 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-4-[(4Z)-4-[[4-(dimethylamino)phenyl]methylene]-2,2-dimethyl-4H-1,3-dioxin-6-yl]-1,3-butadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]C29 H28 N4 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2,2'-[(1E)-1,2-ethenediylbis[(3,4-dibutoxy-5,2-thiophenediyl)-(1E,3E)-1,3-butadiene-4,1-diyl[3-cyano-5-methyl-5-(trifluoromethyl)-4-furanyl-2(5H)-ylidene]]]bis-C54 H52 F6 N6 O6 S2

MF

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-4-(2,6,7,8-tetrahydro-2-methyl-5-isoquinolinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]MF C24 H22 N4 0

Double bond geometry as shown.

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]MF C65 H92 N4 O3 S Si2

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[4-[4-[5-[2-[4-[bis(2-

mercaptoethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-Furanylidene]MF c47 H52 c12 N4 o S3
CC CCM

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[4-[2-[2-[5-[2-[4-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-4-(1-piperidinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]-MF C19 H20 N4 O

Double bond geometry as shown.

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E,3E,5E)-6-(2,6,7,8-tetrahydro-2-methyl-5-isoquinolinyl)-1,3,5-hexatrien-1-yl]-2(5H)-furanylidene]-C26 H24 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2,2'-[(1E)-1,2-ethenediylbis[(3,4-dibutoxy-5,2-thiophenediyl)-(1E,3E)-1,3-butadiene-4,1-diyl(3-cyano-5,5-dimethyl-4-tranyl-2(5H)-ylidene)]]bis-C54 H58 N6 O6 S2

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

ALL ANSWERS HAVE BEEN SCANNED

L3 14 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5-(4-cyclohexylphenyl)-4-[(1E,3E)-4-[5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-5-methyl-2(5H)-furanylidene]MF C53 H64 N4 O S

Double bond geometry as shown.

$$\begin{array}{c|c} \text{Et}_{2N} & \text{NC} & \text{CN} \\ \\ \text{Me} & \text{(CH}_{2})_{5} & \text{Me} & \text{Me} \\ \end{array}$$

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

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FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 STRUCTURE UPLOADED

ABS -- Abstract

IND -- Index Data

PATS -- PI, SO

CAN -- CA Accession Number

STD -- BIB, IPC, and NCL

FIDE - All substance data, except sequence data - FIDE, but only 50 names SQIDE - IDE, plus sequence data SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used - Protein sequence data, includes RN SQD SQD3 - Same as SQD, but 3-letter amino acid codes are used SON - Protein sequence name information, includes RN EPROP - Table of experimental properties PPROP - Table of predicted properties - EPROP, ETAG, PPROP PROP Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

APPS -- Application and Priority Information

IPC -- International Patent Classification

IABS -- ABS, indented, with text labels

BIB -- CA Accession Number, plus Bibliographic Data

L2 L3	0 S L1 14 S L1 FULL
<u>.</u> 4	FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 11 S L3
	FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
<b>1</b> 5	FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 TRA L4 1- RN : 172 TERMS
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L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN

PAGE 1-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

CN Propanedinitrile, 2-[4-[4-[5-[2-[4-[bis(2-

mercaptoethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)
RN 956004-92-5 REGISTRY
ED Entered STN: 27 Nov 2007

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FILE LAST UPDATED: 6 Jun 2010 (20100606/ED)

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s otophore

L8 0 OTOPHORE

=> s optophore

1 OPTOPHORE 1 OPTOPHORES 1 OPTOPHORE

(OPTOPHORE OR OPTOPHORES)

=> d his

L9

L4

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L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 11 S L3

FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010

FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5 TRA L4 1- RN : 172 TERMS FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 L6 172 SEA L5 L7 1 S L3 NOT L6 FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 L8 0 S OTOPHORE L9 1 S OPTOPHORE => s 13 and 19 11 L3 L10 0 L3 AND L9 => s 14 or 19 12 L4 OR L9 => d cbib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 12 ANSWERS - CONTINUE? Y/(N):y

ANSWER 1 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
3:93768 Document No. 152:487904 Strategies for optimizing the
second-order nonlinear optical response in zwitterionic merocyanine dyes.
Teshome, Ayele, Kay, Andrew J.; Woolhouse, Anthony D.; Clays, Koen;
Asselberghs, Inge; Smith, Gerald J. (Department of Chemistry, University
of Leuven, Louvain, B-3001, Belg.). Optical Materials (Amsterdam,
Netherlands), 31(4), 575-582 (English) 2009. CODEN: CMATET. ISSN:
0925-3461. Publisher: Elsevier B.V..
The mol. linear and nonlinear optical (NLO) properties of a series of
seven merocyanine dyes have been studied in solvents covering a broad
range of polarity (dioxane to dimethylsulfoxide). The benchmark for the
series was the "Right hand side" zwitterionic chromophore 1, with a short
conjugation path and 4-pyridinylidene as the donor group. Optimization
strategies to improve the nonlinear response involved an extension of the
conjugation path (with one or two ethenyl groups), annelation (pyridine

quinoline), variation of the solvent polarity and partial ring locking of the x-conjugated system. All chromophores have as the acceptor moiety the cyanodicyanomethylidenedihydrofuran heterocycle. Optimizing the NLO response of these zwitterionic dyes by decreasing the polarity of the solvent is only possible for the parent chromophore 1. This is because the three other successful strategies employed to further improve the second-order NLO response in polar media, result in detrimental aggregation in nonpolar media. 1222190-33-UP 1222190-33-UP RL: PEP (Physical, engineering or chemical process); PRP (Properties);

SPN
(Synthetic preparation); PREP (Preparation); PRCC (Process)
(strategies for optimizing second-order nonlinear optical response in
zwitterionic merocyanine dyes)
RN 122219-03-20 CAPLUS
CN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-4-(2,6,7,8-tetrahydro2-methyl-5-isoquinolinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]THERE MAMP | MAMP |

Double bond geometry as shown.

Lil ANSWER 2 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN 2008:1066476 Document No. 152:64501 2-(3-Cyano-5,5-dimethyl-4-f-(4-(pyrrolidin-1-yl)buta-1,3-dienyl]-2,5-dihydrofuran-2-ylidene|ma|ononitrile dichloromethane solvate. Gainsford, Graeme J.; Bhulyan, M. Delower H.; Kay, Andrew J.; Robinson, Ward T. (Industrial Research Limited, Lower Hutt, N. Z.). Acta Crystallographica, Section E: Structure Reports Online, E64(9), o1715 (English) 2008.

Section E. SCIICODEN:
ACSEBH. ISSN: 1600-5368. URL:
http://journals.iucr.org/e/issues/2008/09/00/lh2664/lh2664.pdf
Publisher:

http://jourman...
Publisher:
Wiley-Blackwell.
AB The structure of the title compound, C18H18N4O-CH2C12, was solved using data collected from a multiple crystal (note high R factors). The crystal structure is dominated by two bifurcated attractive

" N/cvano)

interactions. Crystallog. data are given. 1199786-02-1P

IT

1199786-02-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure of)
1199786-02-1 CAPLUS
Propanedintrile, 2-(3-cyano-5,5-dimethyl-4-[4-(1-pyrrolidinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

L11 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

1222190-33-1 CAPLUS
Propanedinitrile, 2=[3-cyano-5,5-dimethy1-4-[(1E,3E,5E)-6-(2,6,7,8-tetrahydro-2-methy1-5-isoquinoliny1)-1,3,5-hexatrien-1-y1]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN

2008:971112 Document No. 150:248702 A pattern for increasing the first
hyperpolarizability of a push-pull polyene dye as indicated from BTT
calculations. Chafin, Andrew P.; Lindsay, Geoffrey A. (NAVAIR, NAWGWD,
Michelson Laboratory, Chemistry Branch, U.S. Navy, China Lake, CA, 93555,
USA). Polymer Preprints (American Chemical Society, Division of Polymer
Chemistry), 49(2), 991-992 (English) 2008. CODEN: ACPPAY. ISSN:
0032-3934. Publisher: American Chemical Society, Division of Polymer
Chemistry.

AB D. functional theory (DFT) calcns. were performed on a polyene dye
scaffold, keeping the end groups and bridge length the same but varying
the pattern of electron-donating (D) and electron-withdrawing (W)
substituents along the polyene bridge. The basic pattern that increased
the first hyperpolarizability was to place W substituents on
even-numbered
(e) methine carbons, and D substituents on odd-numbered (o) methines
(called the (eWoD) pattern). The numbering scheme used herein for the
dye

scaffold has the #1 methine at the W-terminus of the dye. The {eWoD} pattern polarizes the  $\pi$  bonds along the polyene in the opposite direction that the termini of the dye polarize the dye. By placing cyano and fluorine groups in the {eWoD} pattern along the polyene, a sixfold higher first hyperpolarizability was predicted compared to placing them

the opposite substitution pattern ({oWeD}). A superimposed but weaker gradient pattern was also observed 102705-41-5 RL: PRP (Properties)
(pattern for increasing the first hyperpolarizability of a push-pull polyene dye as indicated from DFT calcns.)
1027095-41-5 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-4-[(4Z)-4-[[4-(dimethylamino)phenyl]methylene]-2,2-dimethyl-4H-1,3-dioxin-6-yl]-1,3-butadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
2008:496216 Document No. 148:563456 A Pattern for Increasing the First
Hyperpolarizability of a Push-Pull Polyene Dye as Indicated from DFT
Calculations. Chafin, Andrew P.; Lindsay, Geoffrey A. (NAVAIR, NAWCWD,
Michelson Laboratory, Chemistry Branch, U.S. Navy, China Lake, CA, 93555,
USA). Journal of Physical Chemistry C, 112(21), 7829-7835 (English)
2008.

CODEN: JPCCCK. ISSN: 1932-7447. Publisher: American Chemical Society. D. functional theory (DFT) calcns, were performed on a polyene dye scaffold, keeping the end groups and bridge length the same but varying the pattern of electron-donating (D) and electron-withdrawing (W) substituents along the polyene bridge. The basic pattern that increased the first hyperpolarizability was to place W substituents on -numbered (e) methine carbons, and D substituents on odd-numbered (o) methines (called the (eWoD) pattern). The numbering scheme used herein for the

scaffold has the #1 methine at the W-terminus of the dye. The {eWoD} pattern polarizes the  $\pi$  bonds along the polyene in the opposite direction that the termini of the dye polarize the dye. By placing cyano and fluorine groups in the {eWoD} pattern along the polyene, a sixfold higher first hyperpolarizability was predicted compared to placing them

the opposite substitution pattern ({oWeD}). A superimposed but weaker gradient pattern was also observed 1027095-41-5 RL: PRP (Properties) (pattern for increasing the first hyperpolarizability of a push-pull polyene dye as indicated from DFT calcns.) 1027095-41-5 CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-4-[(4Z)-4-[4-(dimethylamino)phenyl]methylene]-2,2-dimethyl-4H-1,3-dioxin-6-y1]-1,3-butadien-1-y1]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
2007:1271490 Document No. 147:5030570 Mercaptofunctional high
hyperpolarizability electrooptical chromophores and high glass
temperature, low optical loss, covalently bonded, high
hyperpolarizability
electrooptical chromophore containing polymers and methods of synthesis.
He, Mingdian; Mang, Jianguo (Corning, Inc., USA). U.S. Pat. Appl. Publ.
US 20070257237 Al 20071038, 20 pp. (English). CODEN: USXXCO.
APPLICATION: US 2006-418101 20066093.

AB The present invention relates generally to mercaptofunctional high
μβ EO chromophores and EO polymers, and particularly to
mercaptofunctional high μβ EO chromophores and EO polymers useful
for making electro-optical devices and systems. Mercaptofunctional high
μβ EO chromophore can covalently bonded to poly(imido sulfide)
polymers producing high Tg, low optical loss, covalently bonded, high
μβ EO chromophore containing polymers. Methods of synthesizing these
EO materials using mild polymerization conditions are also described.

IT 956004-93-6P
RL: INF (Industrial manufacture); PRP (Properties); TEM (Technical or
engineered material use); PREP (Preparation); USES (Uses)
(mercaptofunctional high hyperpolarizability electrooptical
chromophores and high glass temperature, low optical loss, covalently
bonded,
high hyperpolarizability electrooptical chromophore containing

bonded, high hyperpolarizability electrooptical chromophore containing

polymers and

mers and
methods of synthesis)
956004-93-6 CAPLUS
Propanedinitrile, 2-[4-[4-[5-[2-[4-[bis(2-

mercaptoethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]-,polymerwith
1,1'-(2,2',3,3',5,5',6,6'-octafluoro[1,1'-biphenyl]-4,4'-diyl)bis[H-pyrrole-2,5-dione] and 4,4'-thiobis[benzenethiol] (CA INDEX NAME)

CM 1

CRN 956004-92-5 CMF C47 H52 C12 N4 O S3

L11 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
2008:148957 Document No. 150:1803140
2-(3-Cyano-5,5-dimethyl-4-(4-(piperidin-1-yl)buta-1,3-dienyl]-2,5-dihydrofuran-2-ylidene|malononitrile. Gainsford, Graeme J.; Bhuiyan, M. Delower H.; Kay, Andrew J.; Spek, Anthony L. (Industrial Research

dihydrofuran-2-ylidene|malononitrile. wainship, and complete the provided of t

Double bond geometry as shown.

L11 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

CM 2

CRN 140714-27-8 CMF C20 H4 F8 N2 O4

L11 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 3

19362-77-7 C12 H10 S3

L11 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

928792-05-6 CAPLUS
Propanedinitrile, 2,2'-[(1E)-1,2-ethenediylbis[(3,4-dibutoxy-5,2-thiophenediyl)-(1E,3E)-1,3-butadiene-4,1-diyl[3-cyano-5-methyl-5-(trifluoromethyl)-4-furanyl-2(5H)-ylidene]]]bis- (CA INDEX NAME)

Double bond geometry as shown.

DAGE 1-A

PAGE 1-B

L11 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN

2007:41926 Document No. 146:3256680 Two-Photon Absorption in Quadrupolar
Bis(acceptor)-Terminated Chromophores with Electron-Rich
Bis(heterocycle)vinylene Bridges. Zheng, Shijun; Leclercq, Amalia; Fu,
Jie; Bewerina, Luca; Padilha, Lazaro A.; Zojer, Egbert; Schmidt, Karin;
Barlow, Stephen; Luo, Jingdong; Jiang, Sei-Hun; Jen, Alex K.-Y.; Yi,
Yuanping; Shuai, Zhigang; Van Stryland, Eric W.; Hagan, David J.; Bredas,
Jean-Luc; Marder, Seth R. (School of Chemistry and Biochemistry, Georgia
Institute of Technology, Atlanta, 68, 30332-0400, USA). Chemistry of
Materials, 19(3), 432-442 (English) 2007. CODEN: CMATEX. ISSN:
0897-4756. OTHER SCURCES: CASREACT 146:325668. Publisher: American
Chemical Society.

AB Two-photon absorption spectra for a range of bis(acceptor)-substituted
bis(dibutoxythienyl)ethene and bis(N-hexylpyrrolyl) ethene chromophores
were recorded using Z-scan and white-light-continuum pump-probe
techniques. All the chromophores studied show strong near-IR two-photon
absorption with cross sections at 2400-5900 CM (1 GM = 1 + 10-50 cm4
s/photon) at photon wavelengths between 1.0 and 1.3 µm; cross sections
≤10000 GM can be accessed close to the 1-photon absorption edge.
Quantum-chemical calcns. reproduce the exptl. observed variations of the
two-photon properties with the chemical structure.

17 928792-03-4P 928792-05-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(two-photon absorption in quadrupolar bis(acceptor)-terminated
chromophores with electron-rich bis(heterocycle) vinylene bridges)

PN 928792-03-4C PAPIUS

CN Propanedinitrile, 2,2'-[(IE)-1,2-ethenediylbis[(3,4-dibutoxy-5,2thiophenediyl)-(1E,3E)-1,3-butadiene-4,1-diyl(3-cyano-5,5-dimethyl-4furanyl-2(SH-yl-Idene)]]bis- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

L11 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN 2005:358523 Document No. 143:777830 Two-Photon Absorption at Telecommunications Wavelengths in a Dipolar Chromophore with a Pyrrole Auxiliary Donor and Thiazole Auxiliary Acceptor. Beverina, Luca; Fu,

Leclercq, Amalia; Zojer, Egbert; Facher, Peter; Barlow, Stephen; Van Stryland, Eric W.; Hagan, David J.; Bredas, Jean-Luc; Marder, Seth R. (School of Chemistry and Biochemistry, Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, GA, 30332-0400, USA). Journal of the American Chemical Society, 127(20), 7282-7283 (English) 2005. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES:

(English) 2005. CASREACT

143:77783. Publisher: American Chemical Society.

AB Three new dipolar chromophores based on a dialkyaminophenyl donor, a pyrrole auxiliary donor, a thiazole auxiliary acceptor, and strong heterocyclic acceptors have been synthesized. For one of these compds.

have measured a very large non-degenerate two-photon cross section of ca. 1500 GM in the near-IR telecommunications range using a pump-probe technique. Calens. indicate the cross section for degenerate two-photon absorption is likely to be ca. 60% of this value. 855774-00-4P

855774-00-4P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (two-photon absorption at telecommunications wavelengths in a dipo chromophore with a pyrrole auxiliary donor and thiazole auxiliary acceptor)
855774-00-4 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[4-[2-[2-[5-[2-[4-

(dibutylamino)phenyl]ethenyl]-1-hexyl-1H-pyrrol-2-yl]ethenyl]-5-thiazolyl]-1,3-butadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

ANSWER 9 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
4:1127374 Document No. 142:745550 A preparation of zwitterionic non-linear [(pyridinylidenealkylene)furanylidene]propanedinitrile derivatives, useful as optical chromophores (optophores).
Woolhouse, Anthony David; Kay, Andrew John (Industrial Research Limited, N. Z.). PCT Int. Appl. Wo 2004111043 A1 20041223, 47 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, 1S, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MM, MK, MN, MM, MX, MZ, NA, NI, NO, NZ, OM, FG, PH, PT, FO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UG, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, TE, IT, LU, MC, MI, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2004-NZ124 20040617. PRIORITY: NZ 2003-526561 20030618.

of

The invention relates to a preparation of zwitterionic second order

linear optophores of formula I (wherein: L is a linking group comprising (un)substituted chain of 3,5, or 7 carbon atoms which, together with the double bond linking D to L forms a conjugated polyenic chain; Rl and R2 are independently selected from alkyl, hydroxyalkyl, or p-C6H4-OAc; D is

heterocycle]. These optophores display a large and efficient non-linear optical response and therefore can be used in the production

optoelectronic devices. For instance, (furanylidene)propanedinitrile derivative II (electronic absorption data in DMF:  $\lambda$ max = 570 nm, log10e = 4.86) was prepared with a yield of 83%.

L11 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

709656-45-1 CAPLUS

Topono-43-1 CAPUS Propanedintrile, cyano-5-(4-cyclohexylphenyl)-4-[(1E,3E)-4-[5-[(1E)-2-[4-(dichylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-5-methyl-2(5H)-furanylidene)- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN 2004:402609 Document No. 141:147753 Photostability of High  $\mu\beta$  Electro-Optic Chromophores at 1550 nm. DeRosa, Michael E.; He, Mingqian; Cites, Jeffrey S.; Garner, Sean M.; Tang, Y. Ruby (Science Technology Division, Corning Incorporated, Corning, NY, 14831, USA). Journal of Physical Chemistry B, 108 (25), 8725-8730 (English) 2004. CODEN: JPCBFK. ISSN: 1520-6106. Publisher: American Chemical Society. AB The authors present the photostability results of seven novel electrooptic chromophores made to be used in high-speed fiber optic signal modulators. The authors measured the photobleaching rate of the chromophores at room temperature by using a fiber optic pump-probe technique. Thin polymer film

temperature by using a fiber optic pump-probe technique. Thin polymer a quest-host samples were deposited on the end of SMF-28 fiber pigtails and bleached by using 100 mW of 1550 mm radiation as the pump. The bleaching rate was measured by monitoring the main absorption band of the chromophores by using a 660. mm probe beam that was multiplexed into the fiber pigtail. The relative photostability is reported as a figure of merit which is proportional to the 1/e bleaching lifetime of the chromophore. The authors found the bleaching rate to increase linearly with incident 1550 mm power at the end of the single-mode fiber up to at least 100 mW. The authors' results show that the photobleaching rate is reduced dramatically when the test is conducted in an inert atmospheric of the presence of the singlet O quencher DABCO can be used to increase the lifetime of the chromophore. The effect that chromophore structure and polymer host type have on photostability are also discussed.

47/892-36-7 70866-45-1 709656-47-3
RL: DEV (Device component use); PRP (Properties); USES (Uses) (photostability of high µB electro-optic chromophores at 1550 mm using in fiber optics modulators)

47/892-36-7 CAPLUS

Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

$$\begin{array}{c} \text{CN} \\ \text{NC} \\ \text{CN} \\ \text{Me} \\ \text{(CH}_2)_{\overline{5}} \end{array}$$

709656-47-3

CN Propanedinitrile,
2-[3-cyano-5-(3,4-dichlorophenyl)-4-[(1E,3E)-4-[5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L11 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

IT 703656-45-1P 703656-47-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of electrooptic chromophores and structure-property relationship)
RN 703656-45-1 CAPLUS
CN Proparadinitrile
2-[3-cyano-5-(4-cyclohexylphenyl)-4-[(1E,3E)-4-[5-[(1E)-2-(4-cidethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 709656-47-3 CAPLUS
Propanedinitrile,
2-[3-cyano-5-(3,4-dichlorophenyl)-4-[(1E,3E)-4-[5-[(1E)-2-(4-diethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L11 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN
2002:787052 Document No. 138:246080 Synthesis of Chromophores with
Extremely
High Electro-optic Activity. 1. Thiophene-Bridge-Based Chromophores. He,
Minggian; Leslie, Thomas M.; Sinicropi, John A. (Corning Incorporated,
Corning, NY, 14831, USA). Chemistry of Materials, 14(11), 4662-4668
(English) 2002. CODEN: CMATEX. ISSN: 0897-4756. OTHER SOURCES:
CASRACT
138:24608. Publisher: American Chemical Society.
AB We have successfully synthesized several new substituted thiophene-based
electro-optic chromophores. All of these chromophores have structures
similar to FTC but they incorporated our newly designed
tricyanovinyldihydrofuran acceptors. Since these acceptors possess an
anisotropic structure, all of the chromophores are very soluble in a wide
range of organic solvents. Thermal study of these chromophores by TGA
shows

all of them are very stable in air. UV spectra indicate the chromophores have a large solvatochromic effect, implying very large mol. nonlinearities.

477892-35-6P 477892-36-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chromophore; synthesis of thiophene-bridge-based chromophores with extremely high electro-optic activity)

477892-35-6 CAPLUS

Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]-1,3-butadien-1-yl]-3cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX
NAME)

Double bond geometry as shown.

477892-36-7 CAPLUS Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

L11 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2010 ACS on STN  $$\operatorname{\textsc{(Continued)}}$$  Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

```
=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
     FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
L1
                STRUCTURE UPLOADED
L2
              0 S L1
L3
             14 S L1 FULL
     FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
             11 S L3
L4
     FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
     FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
                TRA L4 1- RN :
                                    172 TERMS
     FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
            172 SEA L5
L6
              1 S L3 NOT L6
L7
     FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
              0 S OTOPHORE
L9
              1 S OPTOPHORE
L10
              0 S L3 AND L9
L11
             12 S L4 OR L9
     electro-optic chromophores
        102415 ELECTRO
            13 ELECTROS
        102427 ELECTRO
                  (ELECTRO OR ELECTROS)
         69104 OPTIC
         54862 OPTICS
        109521 OPTIC
                  (OPTIC OR OPTICS)
         22778 CHROMOPHORES
            26 ELECTRO-OPTIC CHROMOPHORES
L12
                  (ELECTRO (W) OPTIC (W) CHROMOPHORES)
=> s electroptic chromophores
            25 ELECTROPTIC
             5 ELECTROPTICS
            30 ELECTROPTIC
                  (ELECTROPTIC OR ELECTROPTICS)
         22778 CHROMOPHORES
L13
             0 ELECTROPTIC CHROMOPHORES
                  (ELECTROPTIC (W) CHROMOPHORES)
     electrooptic chromophores
=> s
         10509 ELECTROOPTIC
           872 ELECTROOPTICS
         11072 ELECTROOPTIC
                  (ELECTROOPTIC OR ELECTROOPTICS)
```

22778 CHROMOPHORES

L15

L14 27 ELECTROOPTIC CHROMOPHORES (ELECTROOPTIC(W)CHROMOPHORES)

=> s electrooptic

10509 ELECTROOPTIC 872 ELECTROOPTICS 11072 ELECTROOPTIC

(ELECTROOPTIC OR ELECTROOPTICS)

 $\Rightarrow$  s 115 and chromophore

30266 CHROMOPHORE 22778 CHROMOPHORES 42954 CHROMOPHORE

(CHROMOPHORE OR CHROMOPHORES)

L16 660 L15 AND CHROMOPHORE

=> s 112 or 114 or 116

L17 679 L12 OR L14 OR L16

=> file req

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STRUCTURE FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4 DICTIONARY FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4

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http://www.cas.org/support/stngen/stndoc/properties.html

=> s c6n/rf

L18 269403 C6N/RF

=> s c5n/rf

SYSTEM LIMITS EXCEEDED - SEARCH ENDED

The search profile you entered was too complex or gave too many answers. Simplify or subdivide the query and try again. If you have exceeded the answer limit, enter DELETE HISTORY at an arrow prompt (=>) to remove all previous answers sets and begin at L1. Use the SAVE command to store any important profiles or answer sets before

using DELETE HISTORY.

=> fil tra rn 117

'TRA' IS NOT A VALID FILE NAME

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

ENTER A FILE NAME OR (IGNORE):ignore

'RN' IS NOT A VALID FILE NAME

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

ENTER A FILE NAME OR (IGNORE):end

=> tra rn 117

L19 TRANSFER L17 1- RN : 3023 TERMS

L20 3023 L19

=> s 120 and c5n/rf 7971765 C5N/RF

L21 214 L20 AND C5N/RF

=> d scan 1-

'1-' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

CM 1

CM

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

EPROP - Table of experimental properties PPROP - Table of predicted properties PROP - EPROP, ETAG, PPROP

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when

it is available.

The MAX format is the same as ALL plus SPEC.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCANN (1):end

=> d scan

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4,4'-[[4,5-bis[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsinyl]oxy]ethyl]anino]phenyl]ethenyl]-1,2-phenyleneldi-(1E)-2,1-ethenediyl]bis[1-methyl-, diiodide (9CI)

MF C70 H108 N4 O4 Si4 . 2 I

Double bond geometry as shown.

•2 I-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2000

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 1-(3-hydroxypropyl)-4-methyl-MF C9 H14 N O C1 CCM
- + (СН2)3-ОН

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

D1-Me

CM 2 CM 3

$$\begin{array}{c} \text{HO-CH}_2\text{-CH}_2 \\ \text{HO-CH}_2\text{-CH}_2 \end{array}$$

CM 4

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-(2-carboxyethyl)-4-[2-[4-(didecylamino)phenyl]ethenyl]-, inner salt
MF C36 H56 NZ 02

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 2-Propenoic acid, 2-methyl-, 2-[5-[2-[5,5'-dimethyl-6'-[2-(5-pentyl-2-thienyl)ethenyl][3,3'-bipyridin]-6-yl]ethenyl]-2-thienyl]ethyl ester

MF C35 H38 N2 O2 S2

CI CCM

PAGE 1-A 
$$\begin{matrix} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2,5-Cyclohexadien-1-one,
2,6-bis(1,1-dimethyl)-4-{2-[4-(3,5-dimethyl1-octyl-4(1H)-pyridinylidene)-3,5-dimethyl-2,5-cyclohexadien-1ylidene]ethylidene]MF C39 H55 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 2,5-Cyclohexadien-1-one, 3,5-dimethyl-4-(1,3,5-trimethyl-4(1H)pyridinylidene) 
MF C16 H19 N O
C1 CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Propenoic acid,
2-cyano-3-[5-[5-[4-[(2-methyl-1-oxo-2-propen-1-yl)oxy]1-piperidinyl]-2-thienyl]carbonyl]-2-thienyl]-, ethyl ester, (2E)MF C24 H24 N2 O5 S2
CI CCM

Double bond geometry as shown.

$$\mathsf{Me} \underbrace{\hspace{1cm} \circ \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm} \circ \hspace{1cm} \hspace{1cm} \circ \hspace{1cm} \hspace{1cm} \hspace{1cm} \circ \hspace{1cm} \hspace{1cm$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 4-methyl-1-octyl-, bromide (1:1) MF C14 H24 N . Br

• Br-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1H-Phenanthro[9,10-d] imidazole, 2-(4-nitrophenyl)-6,9-di-1-piperidinylMF C31 H31 N5 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 1-[2-[3,5-bis[(2-ethylhexyl)oxy]phenyl]ethyl]-4-[4(dicyanomethyl)phenyl]-, inner salt

MF C38 H49 N3 02

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN No. Pyridinium, 4-(4-methoxy-2,6-dimethylphenyl)-1,3,5-trimethyl-, iodide (1:1) MF C17 H22 N O . I

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E,3E)-4-[4-(dimethylamino)phenyl]-1,3-butadien-1-yl]-1phenylMF C23 H23 N2
CI CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 9H-Fluoren-2-amine, 9,9-didecyl-N,N-diphenyl-7-[2-(4-pyridinyl)ethenyl]MF C52 H64 N2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1-Propanol, 3,3\*-[[4-(4-pyridinylethynyl)phenyl]imino]bis- (9CI)
MF C19 H22 N2 O2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[2-[4-(dimethylamino)phenyl]=thenyl]-1-ethyl-, iodide (1:1)
MF C17 H21 N2 . I

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
4-anino-1-naphthalenezulfonate (1:1)

MF C16 H19 N2 .C10 H8 N O3 S

CM 1

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Piperidinecarbonitrile,
5-[2-(1-butyl-1,3-dihydro-3,3-dimethyl-2H-indol2-ylidene)ethylidene]-1-(2-ethylhexyl)-4-methyl-2,6-dioxoMF C31 H43 N3 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]=thenyl]-1-phenylMF C21 H21 N2
CI CCM

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(1-piperidiny1)MF C14 H15 N O S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 2-chloro-3,5-dinitro-MF C5 H2 Cl N3 O4 CI CM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 1-methyl-4-[2-(1-pyrenyl)ethenyl]-, (E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C24 H18 N . C7 H7 O3 S

Double bond geometry as shown.

CM 1

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium,
4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]1-(2-hydroxyethyl)-, inner salt

MF C20 H17 N3 O3

$$\begin{array}{c|c} & \text{CN} & \\ & \text{CH} & \text{CH} & \\ & \text{HO-CH}_2-\text{CH}_2 \end{array}$$

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)oxy-1,4-phenylene(1-

methylethylidene)-1,4-phenyleneoxy(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)-1,4-phenyleneoxy(5-carboxy-1,3-phenylene)oxy-1,4-phenylene],

\[ \alpha - (4-[3-carboxy-5-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl) phenoxy] phenyl)-\alpha - (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-, 3,5-bis(1,1-dimethylethyl)phenyl ester, ester with

\[ \alpha - ((12)-2-cyano-2-[4-(dicyanomethyl)phenyl ethenyl]-1-(3-hydroxyproyxl) pyridinium inner salt (9C1)
\]

MF ((C50 H32 N2 O10)n C35 H20 N2 O8 . x C20 H16 N4 O . x C14 H22 O

CM 1

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PAGE 1-B

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued) PAGE 1-C

CM 2

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[5-[2-[4-(diphenylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]MF C33 H18 F4 N4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 4,6(1H,5H)-Pyrimidinedione, 1,3-diethyldihydro-5-[[5-(1-piperidinyl)-2-thienyl]methylene]-2-thioxo
MF C18 H23 N3 O2 S2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E,3E)-4-(4-methoxyphenyl)-1,3-butadienyl]-1-methyl-,
salt

salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C17 H18 N O . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
Pyridinium, 4-[4-[(1E)-2-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethenyl]-2,6-dimethylphenyl]-3,5-dimethyl-1-octyl-MF C39 H56 N O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-methyl- MF C6 H7 N C C0M

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[[4-[(1E)-2-(2,6-diamino-4-pyridinyl)ethenyl]methylene]MF C18 H15 N5 03

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Piperidine,
1-[5'-[(1E)-2-[2,2'-bithiophen]-5-yletheny1][2,2'-bithiophen]MF C23 H21 N S4

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]-MF C11 H9 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-1-methyl, 4-methylbenzenesulfonate (1:1)
MF C22 H27 N2 04 . C7 H7 03 S

CM 2

CM 1

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]1-(3-hydroxypropyl)-, inner salt
MF C21 H19 N3 O3

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]
MF C28 H37 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Thiophenecarboxaldehyde, 5-[[5-(4-hydroxy-1-piperidinyl)-2-thienyl]carbonyl]MF C15 H15 N O3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(12)-2-cyano-2-[4-(dicyanomethyl)phenyl]ethenyl]-1-octyl-,
inner salt
MF C25 E126 N4

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[4-(1-piperidinyl)phenyl]methylene]MF C15 H15 N3
C1 COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenamine, 4-(3,5-dimethyl-4-pyridinyl)-N-(diphenylmethylene)-3,5-dimethyl
MF C28 H26 N2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
4-[2-[4-(dimethylamino)phenyl]diazenyl]benzenesulfonate (1:1)
MF C16 H19 N2 .C14 H14 N3 O3 S

CM 1

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1,1'-(dithiodi-11,1-undecanediy1)bis[4-[2-[4-(dibtylamino)phenyl]ethenyl]-, bromide (1:2)
MF C64 H100 N4 S2 . 2 Br

●2 Br-

PAGE 1-B

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Acetonitrile, 2-(2,6-dimethyl-4(1H)-pyridinylidene)-MF C9 H10 N2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2,6-Pyridinediamine, 4-(phenylmethoxy)-MF C12 H13 N3 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

NPyridinium, 4-[(1E,5E,5E)-6-[4-(dimethylamino)phenyl]-1,3,5-hexatrien-1-yl]-1-methyl-, 4-methylbenzenesulfonate (1:1)

MF C20 H23 N2 . C7 H7 O3 S

CM 1

Double bond geometry as shown.

CM 2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[2,5-bis(1-methylethyl)-4-(1-piperidinyl)phenyl]methylene]MF C21 H27 N3

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-y-methyl-,
3-[4-[2-cyano-2-(4-dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1(4H)-pyridinyl]propyl ester, polymer with
1,3,5-benzenetricarbonyl trichloride (9C1)

MF (C37 H32 N4 O4 . C9 H3 Cl3 O3)x

CI PMS

CM 1

CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Hexanamide, N,N'-(4-hydroxy-2,6-pyridinediyl)bis-MF C17 H27 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Ethanol,
2,2'-[[4-[[2-(4-pyridinyl)-6-benzothiazolyl]azo]phenyl]imino]bis(901)
MF C22 H21 N5 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 3-methyl-4-nitro-, 1-oxide MF C6 H6 N2 O3 C COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1N 2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dibutyl-5-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]
MF C20 H27 N3 03

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Hexanamide, N,N',N''',N'''-[[[4-[2-(5-formyl-2-thlenyl)]phenyl]jmino]bis(2,1-ethanediyloxy-4,2,6-pyridinetriyl)]tetrakis- (9CI)

MF C51 H69 N7 O7 S

PAGE 1-A

PAGE 1-B

- (CH2)4-Me

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Piperidine, 1-(5'-nitro[2,2'-bithiophen]-5-y1)MF C13 H14 N2 O2 S2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2-Propenoic acid, 2-methyl-, 2-(9H-carbazol-9-yl)ethyl ester, polymer with

2-[5-[2-[5,5'-dimethyl-6'-[2-(5-pentyl-2-thienyl)ethenyl][3,3'-bipyridin]-6-yl]ethenyl]-2-thienyl]ethyl 2-methyl-2-propenoate
MF (C35 H38 N2 O2 S2 . C18 H17 N O2)x
CT PMS

CM 1

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
1-(2-carboxyethyl)-4-[2-[4-(dioctadecylamino)phenyl]ethenyl]-,
inner salt
MF C52 H88 N2 O2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Pyridinium,
4-[4-[2-[4-(dicyanomethyl)phenyl]ethenyl]-2,6-dimethylphenyl]3,5-dimethyl-1-(2-propylheptyl)-, inner salt

MF C36 H43 N3

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[10-[4-(dihexylamino)phenyl]-1,3,5,7,9-decapentaen-1-yl]-1-(4-sulfobutyl)-, inner salt
NF C37 H52 W2 O3 S

PAGE 1-A

PAGE 1-B

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

NPyridinium,
4-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-1-butyl, tetraphenylborate(1-), polymer with silicic acid (#48i04) tetraethyl
ester and triethoxy(3-isocyanatopropyl)silane (9CI)

MF (C24 H20 B . C21 H29 N2 O2 . C10 H21 N O4 Si . C8 H20 O4 Si)x

CI PMS

CM 1

CM 2

м 3

 $$\operatorname{\textsc{CM}}$$  -4 Double bond geometry as shown.

CM 5

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Dibenzo[a,c]phenazine, 11-nitro-3,6-di-1-piperidinyl-MF C30 H29 N5 O2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Piperidine, 1-[4-[2-(4-nitrophenyl)diazenyl]phenyl]-MF C17 H18 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-(4-iodo-2,6-dimethylphenyl)-3,5-dimethylmF C15 H16 I N

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 2-Propenoic acid, 2-methyl-, 2-[4,4'-dimethyl-5'-[2-(5-methyl-2-thienyl)ethenyl][2,2'-bipyridin]-5-yl]ethyl ester

MF C25 H26 N2 O2 S
CI COM

Me CH=CH=CH=
$$^{\circ}$$
 CH= $^{\circ}$  CH2-CH2-O-C-C-M

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Methanone, [5-(1-piperidiny1)-2-thieny1]-2-thieny1-MF C14 H15 N O S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-(4-bromophenyl)MF C11 H8 Br N C1 COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2,2':6',2''-Terpyridine, 4'-bromo-MF C15 H10 Br N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium,  $4-[(1E)-2-[4-(\dim \operatorname{thylamino})\operatorname{phenyl}] = 1-\operatorname{methyl-}, 2, 4, 6-\operatorname{trimethylbenzenesulfonate} (1:1)$  MF C16 H19 N2 . C9 H11 O3 S

CM 1

Double bond geometry as shown.

CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridine, 4-(4-methoxy-2,6-dimethylphenyl)-3,5-dimethylMF C16 H19 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

CM 1

CM 2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-(2-pyrimidinyl)MF C19 H19 N4
CI CCM

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-methyl-4-(6-ruthenocenyl-1,3,5-hexatrienyl)-, (E,E,E)-,
salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C22 H22 N Ru . C7 H7 O3 S CM 1

PAGE 1-A

PAGE 2-A

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2-Pyridinamine, 5-nitroMF C5 H5 N3 O2
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 1-[3-[[4,4-bis(4-hydroxyphenyl)-1-oxopentyl]oxy]propyl]-4methylMF C26 H30 N O4
CI CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4,4'-[[4,5-bis[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl-dimethylamino]phenyl]ethenyl]-1,2-phenylene]di-(1E)-2,1-ethenediyl]bis[1-methyl-, salt with trifluoromethanesulfonic acid (1:2) (9CI)

MF C70 H108 N4 O4 Si4 . 2 C F3 O3 S

CM 1

Double bond geometry as shown.

PAGE 1-A t-Bu Si Me Me

PAGE 2-A

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4,4'-[(1-methyl-1H-pyrrole-2,5-diyl)di-2,1-ethenediyl]bis[1-methyl- (9CI) H23 N3
CI CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Proparedinitrile, 2-[3-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]-2-propen-1-ylidene]NF C21 H19 N3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 4-[2-(2,4-dimethoxyphenyl)ethenyl]-1-methyl-, (E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C16 H18 N O2 . C7 H7 O3 S

CM 1

Double bond geometry as shown.

CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Piperidine NF C5 H1 N C COM, RPS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN NP pyridinium, 1-methyl-4-[2-[1-methyl-5-[2-(4-pyridinyl)ethenyl]-1H-pyrrol-2-yl]ethenyl] 
MF C20 H20 N3 CT CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 4-[(1E)-2-[4-[(1E)-2-[4-[bis[2-[[(1,1-

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Hexanamide, N,N',N'',N'''-[[[4-[(4-nitrophenyl)azo]phenyl]imino]bis(2,1-ethanediyloxy-4,2,6-pyridinetriyl)]tetrakis- (9CI)

MF C50 H68 N10 08

PAGE 1-B

-- NO2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-1-methyl-,
tetrafluoroborate(1-) (1:1)

MF C18 H23 N2 02 . B F4

CI CCM

CM 1

$$\begin{array}{c} \text{Me} \\ \text{HO-CH}_2\text{-CH}_2 \\ \text{HO-CH}_2\text{-CH}_2 \end{array}$$

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 2-Thiophenethanol, 5-[2-[5,6'-dimethyl-6'-[2-(5-pentyl-2-thienyl)ethenyl]], 3'-bipyridin]-6-yl]ethenyl]
MF C31 H34 N2 0 S2

PAGE 1-B

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

TN Pyridinium, 1-(2-carboxyethyl)-4-[2-[4-(dihexylamino)phenyl]ethenyl]-,
inner salt

MF C28 H40 N2 O2

$$\begin{array}{c} \text{Me} - (\text{CH}_2) \text{ 5} \\ \text{Me} - (\text{CH}_2) \text{ 5} - \text{N} \\ \end{array}$$

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]ethylidene]-2,5-cyclohexadien-1-ylidene]
MF C36 H43 N3

<sup>\*\*</sup>PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-(3-hydroxypropyl)-4-methyl-, bromide (1:1)
MF C9 H14 N O . Br

• Br -

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

2-Propenoic acid, 2-cyano-3-[5-[5-(4-hydroxy-1-piperidinyl)-2-thienyl]carbonyl]-2-thienyl]-, ethyl ester, (2E)
MF C20 H20 N2 O4 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-bromo-3,5-dimethyl-, 1-oxide MF C7 H8 Br N O C COM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[4-(dicyanomethyl)phenyl]-1-(2-propylheptyl)-, inner salt
MF C24 H29 N3

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-(4-hydroxy-2,6-dimethylphenyl)-1,3,5-trimethyl-, iodide
(111)
MF C16 H20 N O . I

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Zinc,
[5,15-bis[2,6-bis(3,3-dimethylbutoxy)phenyl]-10,20-bis([2,2':6',2''-terpyridin]-4'-ylethynyl)-21H,23H-porphinato(2-)
KN21,KN22,KN23,KN24]-, (SP-4-1)- (9CI)

MF C90 H86 N10 04 Zn

CI CCS

PAGE 1-A

$$\begin{array}{c} \text{Me}_{3}\text{C-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{O} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{Me}_{3}\text{C-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{O} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{O} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CMe}_{3} \\ \text{CH}_{2}\text{-}\text{CH}_{2}\text{$$

PAGE 1-B

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN 4,6(1H,5H)-Pyrimidinedione, 1,3-diethyldihydro-5-[3-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]-2-propen-1-ylidene]-2-thioxo-MF C26 H29 N3 O2 S3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2-Pyridinamine, 5-nitro-, phosphate (1:1) MF C5 H5 N3 O2 . H3 O4 P

CM 1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4=[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
1-naphthalenesulfonate (1:1)

MF C16 H19 N2 . C10 H7 03 S

CM 1

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 2-ethenyl-, homopolymer (C7 H7 N)x CP PMS, COM

CM 1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Noly [oxycarbonyl-1,3-phenylenecarbonyloxy-1,4-phenylene[4-[3-[4-[2-cyano-2[4-(dicyanomethylene)-2,5-cyclohexadien-1-ylidene]ethylidene]-1(4H)pyridinyl]propoxy]-1-methyl-4-oxobutylidene]-1,4-phenylene] (9CI)

GI PMS

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[6-[2-[4-[bis[2-[[(1,1dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]diazenyl]-2benzothiazolyl]-1-[3-(trimethoxysilyl)propyl]-, iodide (1:1)

MF C40 H64 N5 O5 S si3 . I

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1-Propanol, 3,3'-[[4-[2-(4-pyridiny1)etheny1]pheny1]imino]bisMF C19 H24 N2 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-1-butyl, tetraphenylborate(1-) (9CI)
MF C24 H20 B . C21 H29 N2 O2
CI CCM CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Boronic acid, B-4-pyridinyl- MF C5 H6 B N O2 CI CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Pyridinium, 1-[3-[(4,4-bis(4-hydroxyphenyl)-1-oxopentyl]oxy]propyl]-4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]-, inner salt

MF C38 H35 N3 O6

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Benzoic acid, 3,5-bis(4-aminophenoxy)-, polymer with

5,5'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[1,3isobenzofurandione], 3,5-bis(1,1-dimethylethyl)phenyl ester, ester with

4-[(12)-2-cyano-2-[4-(dicyanomethyl)phenyl]ethenyl]-1-(3hydroxyproyl)pyridinium inner salt (9CI)

MF (C31 H20 O8 . C19 H16 N2 O4)x . x C20 H16 N4 O . x C14 H22 O

CM 1

Double bond geometry as shown.

3 CM

CM 4

CM 5

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[[5-[2-[4-(dibutylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]
MF C29 H26 F4 NN4 S

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,1,2-Ethenetricarbonitrile, 2-[5'-(1-piperidinyl)[2,2'-bithiophen]-5-yl]-MF C18 H14 W4 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-ethenyl-MF C7 H7 N C C C C C C  $^{\prime\prime}$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN NPyridinium, 4-[2-(4-methoxyphenyl)ethenyl]-1-methyl-, (E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C15 H16 N O . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[4-[(1E)-2-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethenyl]-2,6-dimethylphenyl]-3,5-dimethyl-1-octyl-, iodide (1:1)

MF C39 H56 N O . I

Double bond geometry as shown.

$$\begin{array}{c} \text{T-Bu} \\ \text{OH} \\ \text{Me} \\ \text{(CH2)} \\ \text{N} \end{array}$$

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Propenoic acid, 2-methyl-, 2,2,2-trifluoroethyl ester, polymer with
4-ethenylpyridine (9CI)
MF (C7 H7 N . C6 H7 F3 02)x
CI PMS

CM 1

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 4,6(1H,5H)-Pyrimidinedione, 1,3-diethyldihydro-5-[3-[5-(1-piperidinyl)-2-thienyl]-2-propen-1-ylidene]-2-thioxoMF C20 H25 N3 O2 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 1-hexyl-4-methyl-MF C12 H20 N C C C M

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-[[4-(hydroxymethyl)phenyl]methyl]-4-methylMF C14 H16 N O

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3,5-dimethyl-4-(1,3,5-trimethyl-4(1H)-pyridinylidene)-2,5-cyclohexadien-1-ylidene]-C19 H19 N3 CC CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4,4'-[(1-methyl-1H-pyrrole-2,5-diyl)di-2,1-ethenediyl]bis-(9CI) MF C19 H17 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Thiophenecarboxaldehyde, 5-[[5-(1-piperidiny1)-2-thieny1]carbony1]MF C15 H15 N O2 S2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 6-Benzothiazolamine, 2-(4-pyridinyl)- MF C12 H9 N3 S C COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 4-methyl-1-(phenylmethyl) - CI3 H14 N C COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
4-(phenylamino)benzenesulfonate (1:1)
MF C16 H19 N2 . C12 H10 N O3 S

CM 1

Double bond geometry as shown.

CM 2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN N Phenol, 2,6-bis(1,1-dimethylethyl)-4-[(1E)-2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]ethenyl]- MF C31 H39 N O

Double bond geometry as shown.

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)pyridinylidene]ethylidene]-2(5H)-thienylidene]MF C21 H24 N4 O2 S
C1 CCM

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{OH} \\ \text{CM} \\ \text{NC}-\text{CS} \\ \text{CH}-\text{CH} \\ \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenamine,
N,N-bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-4-[2(4-pyridinyl)diazenyl]MF C27 H46 N4 O2 Si2

$$\begin{array}{c} \text{Me} \\ \text{t-Bu-si-O-CH}_2\text{-CH}_2\text{-N} \\ \text{Me} \end{array} \begin{array}{c} \text{Me} \\ \text{CH}_2\text{-CH}_2\text{-O-Si-Bu-t} \\ \text{Me} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium,  $4-[2-(3,4-{\rm dihydroxyphenyl}){\rm ethenyl}]-1-{\rm methyl}-$ , (E)-, salt with  $4-{\rm methyl}{\rm benzenesulfonic acid}$  (1:1) (9CI) MF C14 H14 N O2 . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)-MF C9 H7 N3



L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[2,5-diethyl-4-(1-piperidinyl)phenyl]methylene]MF C19 H23 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Ethanol, 2,2'-[[2-(4-pyridinyl)-6-benzothiazolyl]imino]bisMF C16 H17 N3 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenebutanoic acid, 4-hydroxy-γ-(4-hydroxyphenyl)-γ-methyl-,
3-bromopropyl ester, compd. with 4-methylpyridine (1:1) (9CI)

MF C20 H23 Br O4 . C6 H7 N

CM 1

CM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 5(4H)-Isoxazolone, 3-phenyl-4-[3-[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thienyl]-2-propen-1-ylidene]- MF C27 H24 N2 O2 S2

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Pyridinium, 4-[2-(4-bromophenyl)ethenyl]-1-methyl-, (E)-, salt with

4-methylbenzenesulfonic acid (1:1) (9CI)

NF C14 H13 Br N . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[5-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]-4phenyl-2(5H)-thiazolylidene]
MF C20 H14 N4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzenamine, N,N-dimethyl-4-[2-(4-pyridinyl)ethenyl]-MF C15 H16 N2 C COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Pyridinium, 1-methyl-4-[2-[1-methyl-5-[[1-methyl-5-[2-(4-pyridinyl)ethenyl]-1H-pyrrol-2-yl]methyl]-1H-pyrrol-2-yl]ethenyl]
MF C26 H27 N4
C1 C0M

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Hexanamide, N,N',N'',N'''-[[[4-[2-[5-[(1,3-diethylterahydro-4,6-dioxo-2-thioxo-5(2H)-pyrimidinylidene)methyl]-2-thienyl]ethenyl]phenyl]imino]bis(2,1-ethanediyloxy-4,2,6-pyridinetriyl)]tetrakis- (9CI)

MF C59 H79 N9 08 S2

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
1-(2-carboxyethyl)-4-[2-[4-(ditetradecylamino)phenyl]ethenyl], inner salt
MF C44 H72 N2 O2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Hexanamide, N,N'-[4-(phenylmethoxy)-2,6-pyridinediyl]bisMF C24 H33 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Propenoic acid, 2-methyl-, 2-[5-[2-[5,5"-dimethyl-6"-[2-(5-pentyl-2-thienyl)ethenyl][3,3"-bipyridin]-6-yl]ethenyl]-2-thienyl]ethyl ester, homopolymer
MF (G35 H38 N2 O2 S2)x
CI FMS

CM

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[4-(dicyanomethyl)-2,6-dimethylphenyl]-3,5-dimethyl-1-(2-propylheptyl)-, inner salt

MF C28 H37 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1H-Pyrrole-2-carboxaldehyde, 1-methyl-5-[2-(4-pyridinyl)ethenyl]MF C13 H12 N2 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 2-Propenoic acid, 2-cyano-3-[5-[5-[4-[(2-methyl-1-cxo-2-propenyl)cxy]-1-piperidinyl]-2-thienyl](actronyl)-2-thienyl], ethyl ester, (E)-, polymer with 11-(9H-carbarol-9-yl)undecyl 2-methyl-2-propenoate (9CI)

CI PMS

CF PMS

CM 1

Double bond geometry as shown.

$$\begin{array}{c|c} ^{\rm H_2C} & \circ \\ \parallel & \parallel \\ {\rm Me} - {\rm C} - {\rm C} - {\rm O} - ({\rm CH_2})_{11} \\ \end{array}$$

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Methanone, [2,3-bis[4-(1-piperidinyl)phenyl]-6-quinoxalinyl]phenylMF C37 H36 N4 O

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[(1E)-2-(4-(dimethylamino)phenyl]-1-methyl-, salt with 4-methylbenzenesulfonic acid (1:1)

MF C16 H19 N2 . C7 H7 O3 S

CI CCM

CM 1

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN IN Methanesulfonic acid, 1,1,1-trifluoro-, 4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl ester MF C16 H16 F3 N O3 S

$$F_{3}C-\underset{\bigcirc}{\overset{\text{Me}}{=}}\underset{\text{Me}}{\overset{\text{Me}}{=}}\underset{\text{Me}}{\overset{\text{Me}}{=}}\underset{\text{Me}}{\overset{\text{N}}{=}}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN [2,2"-Bipyridine]-5-ethanol, 4,4'-dimethyl-5'-[2-(5-methyl-2-thienyl)ethenyl]
NF C21 H22 N2 0 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E,3E)-4-[4-(dimethylamino)phenyl]-1,3-butadien-1-yl]-1(2,4-dinitrophenyl)MF C23 H21 N4 O4
CI CCM

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine, 4-[2-(1-methyl-1H-pyrrol-2-yl)ethenyl]-MF C12 H12 N2 C1 COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Lithium, (2,3,5,6-tetrafluoro-4-pyridinyl)- MF C5 F4 Li N CI CCM

$$F$$
 $N$ 
 $F$ 
 $F$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Pyridinamine, 5-mitro-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
MF C5 H5 N3 O2 . C4 H6 O6

CM 1

CM 2

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
2-naphthalenesulfonate (1:1)

MF C16 H19 N2 .C10 H7 O3 S

CM 1

Double bond geometry as shown.

CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridine, 4-(4-methoxy-2,6-dimethylphenyl)-3,5-dimethyl-, 1-oxide
MF C16 H19 N O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[2-[4-[bis(9,9-diethoxy-4-oxo-3,10-dioxa-5-aza-9-siladodec-1-y1)amino]phenyl]ethenyl]-1-butyl-, (E)-, tetraphenylborate(1-) (9CI)
MF C41 H71 N4 010 Si2 . C24 H20 B

CM 1

Double bond geometry as shown.

CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-(2,4-dinitrophenyl)WF C21 H19 N4 O4
CI CCM

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-(6-ferrocenyl-1,3,5-hexatrienyl)-1-methyl-, (E,E,E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI)

MF C22 H22 Fe N . C7 H7 O3 S

CM 1

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 2-Pyridinamine, 3-nitro-MF C5 H5 N3 O2 CT COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium,
4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]1-(phenylmethyl)-, inner salt
MF C25 H19 N3 O2

$$\begin{array}{c} \text{CN} \\ \text{Ph-CH2} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzenamine, 4, 44-[4,5-bis[(1E)-2-(4-pyridinyl)ethenyl]-1,2-phenylene]diditle. (1E)-2,1-ethenediyl]bis[N,N-bis[2-[[(1,1-dimethylethyl]dimethylsilyl]oxy]ethyl]- (9CI) MF C68 H102 N4 O4 Si4

Double bond geometry as shown.

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L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, [[5-[2-[4-[bis(butylphenyl]amino]phenyl]ethenyl]-2-thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]- (9CI)

MF C41 H34 F4 N4 S

CI IDS

2 (D1-Bu-n)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]methylene]MF C19 H17 N3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-methyl-4-[2-[4-(methylthio)phenyl]ethenyl]-, (E)-, salt
with

4-methylbenzenesulfonic acid (1:1) (9CI)
MF C15 H16 N S . C7 H7 O3 S

CM 1

Double bond geometry as shown.

CM 2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridine MF C5 H5 N CI CCM, RPS



L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 4-[(1E)-2-[4-[(1E)-2-[4-[bis[2-[[(1,1-

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,1,2-Ethenetricarbonitrile, 2-[5'-[(1E)-2-[5'-(1-piperidiny1)[2,2'-bithhophen]-5-y1]etheny1][2,2'-bithiophen]-5-y1]- MF C28 H20 N4 S4

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1N 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[[4-[(1E)-2-(2,6-diamino-3-pyridinyl)ethenyl]phenyl]methylene]
MF C18 H15 N5 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-1-methyl-,
4-methylbenzenesulfonate (1:1)

MF C18 H23 N2 02 . C7 H7 03 S

CI COM

CM 1

CM 2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[2-[4-(dimethylamino)phenyl]=thenyl]-1-docosyl-, bromide
(1:1)
MF C37 H61 N2 . Br
CI CCM

• Br-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]phenyl]MF C26 H23 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

NPyridinium,
4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]1-[4-(hydroxymethyl)phenyl]methyl]-, inner salt

MF C26 H21 N3 O3

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[(12)-2-cyano-2-[4-(dicyanomethyl)phenyl]ethenyl]-1-(3-hydroxypropyl)-, inner salt

MF C20 H16 N4 O

CC CCM

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

2-Propenoic acid, 2-cyano-3-[5-[[5-(1-piperidiny1)-2-thieny1]carbony1]-2-thieny1]-, ethy1 ester, (2E)
MF C20 H20 N2 03 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Quinoxaline, 6-nitro-2, 3-bis[4-(1-piperidinyl)phenyl]MF C30 H31 N5 02

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-, iodide
(1:1)
MF C16 H19 N2 . I
CI CCM

Double bond geometry as shown.

• I-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-(4-pyridiny1)pheny1]-, ion(1-), sodium (1:1) MF C14 H8 N3 . Na

• Na+

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenamine, 4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylMF C15 H18 N2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Zinc, [5,15-bis[2,6-bis(3,3-dimethylbutoxy)phenyl]-10-(2-[2,2':6',2''-terpyridin]-4'-vylethynyl)-21H,23H-porphinato(2-)
KN21, KN22, KN23, KN24]-, (SP-4-2)
GC 73 H77 N7 04 Zn

CT CCS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 4,6(1H,5H)-Pyrimidinedione, 1,3-diethyldihydro-5-[3-[5-[2-[4-(1-piperidinyl)phenyl]ethenyl]-2-thienyl]-2-propen-1-ylidene]-2-thioxo-MF C28 H31 N3 O2 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium, 1-docosyl-4-[2-(4-hydroxyphenyl)ethenyl]-, bromide (1:1) MF C35 H56 N O . Br

• Br -

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
4-methylbenzenesulfonate (1:1)
MF C16 H19 N2 . C7 H7 O3 S

CM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium,  $4-[(1E)-2-[4-(\dim ethylamino)phenyl] = 1-methyl-, 2,4-dimethylbenzenesulfonate (1:1) MF C16 H19 N2 . C8 H9 O3 S$ 

CM 1

CM 2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzenamine, N,N-bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-4-[2-[2-(4-pyridinyl)-6-benzothiazolyl]diazenyl]-MF C34 H49 N5 O2 S Si2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,1,2-Ethenetricarbonitrile, 2-[2-[5-(1-piperidiny1)-2-thieny1]-2-thieny1]- MF C20 H16 N4 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 4-Pyridinamine, N,N-dimethyl- C7 H10 N2 CC CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[(1E, 3E)-4-[4-(dimethylamino)phenyl]-1,3-butadien-1-yl]-1methyl-, 4-methylbenzenesulfonate (1:1)

MF C18 H21 N2 . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Pyridinium,
4-[2-cyano-2-[4-(1-cyano-2-methoxy-2-oxoethyl)phenyl]ethenyl]1-hexyl-, inner salt
MF C24 H25 N3 O2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)oxy-1,4-phenylene(1-

methylethylidene)-1,4-phenyleneoxy(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)-1,4-phenyleneoxy(5-carboxy-1,3-phenylene)oxy-1,4-phenylene],3,5-bis(1,1-dinethylethyl)phenyl ester, ester with 4-[(12)-2-cyano-2-[4-(dicyanomethyl)phenyl]ethenyl]-1-(3-hydroxypropyl)pyridinium inner salt (9CI)
MF (C50 H32 N2 O10)n . x C20 H16 N4 O . x C14 H22 O

CM 1

PAGE 1-A

PAGE 1-B

CM 2

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[2-[4-[bis[2-[[(1,1dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]diazenyl]-1-[3(trimethoxysilyl)propyl]-, iodide (1:1)

MF C33 H61 N4 O5 Si3 . I

$$\begin{array}{c} \text{Me} \\ \text{t-Bu-} \\ \text{Si-} \\ \text{O-} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{O-} \\ \text{Si-} \\ \text{Bu-} \\ \text{Me} \\ \end{array}$$

• I-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[[5'-(1-piperidiny1)[2,2'-bithiophen]-5-y1]methylene]-MF C17 H15 N3 S2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-methyl-4-[2-(1-methyl-1H-pyrrol-2-yl)ethenyl]MF C13 H15 N2
CI CCM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 4-Pyridinecarboxylic acid MF C6 H5 N O2 CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN N Pyridine, 4-[2-(1-methyl-1H-pyrrol-2-yl)ethenyl]-, mono(tetrafluoroborate(1-)] (9CI) MF C12 H12 N2 . B F4 . H

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[2-[4-(dihexylamino)phenyl]ethynyl]-1-(4-sulfobutyl)-,
inner
salt
MF C29 H42 N2 O3 S

Me
$$^{-}$$
 (CH<sub>2</sub>)<sub>5</sub> $^{-}$  N  $^{+}$  (CH<sub>2</sub>)<sub>4</sub> $^{-}$  SO<sub>3</sub> $^{-}$  Me $^{-}$  (CH<sub>2</sub>)<sub>5</sub>

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Pyridinium, 4-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-1-methyl-, salt with 4-methylbenzenesulfonic acid (1:1), polymer with silicic acid (H4SiO4) tetraethyl ester and triethoxy(3-isocyanatopropyl)silane (9CI)

NF (C18 H23 N2 O2 . C10 H21 N O4 Si . C8 H20 O4 Si . C7 H7 O3 S)x

CI PMS

CM 1

CM 2

CM

CM 4

CM 5

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, [[5-[2-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]etheny1]-2-thieny1]methylene]-, (E,E)- (9CI)

MF C25 H21 N3 S3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 4-Pyridinamine, N,N-dimethyl-, 4-methylbenzenesulfonate (1:1)
MF C7 H10 N2 . C7 H8 O3 S

CM 1

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2-Propenoic acid, 2-methyl-, 2-(9H-carbazol-9-yl)ethyl ester, polymer with

2-[4,4'-dimethyl-5-[2-(5-methyl-2-thienyl)ethenyl][2,2'-bipyridin]-5-yl]ethyl 2-methyl-2-propenoate (C25 H26 N2 O2 S . C18 H17 N O2)x PMS

CM 1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridine, 4,4'-[methylenebis[(1-methyl-1H-pyrrole-5,2-diyl)-2,1-ethenediyl]]bis- (9CI)
MF C25 H24 N4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]MF C18 H17 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Methanone, [5-(4-hydroxy-1-piperidiny1)-2-thieny1]-2-thieny1MF C14 H15 N O2 S2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Piperidine, 1,1'-[(2-(4-nitrophenyl)-1H-imidazole-4,5-diyl]di-4,1-phenylene]bis- (9CI)

MF C31 H33 N5 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-(2-carboxyethyl)-4-methyl-, bromide (1:1)
MF C9 H12 N O2 . Br

● Br -

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 4-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-1-methyl-,
4-ethenylbenzenesulfonate (1:1)
MF C16 H19 N2 . C8 H7 O3 S

CM 1

Double bond geometry as shown.

CM 2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN N Phenol, 4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethyl-MF C15 H17 N O

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Pyridinium, 1-(4-methoxyphenyl)-2,4,6-triphenyl-, tetrafluoroborate(1-)
MF C30 H24 N O . B F4

CM 1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Pyridinium, 4-[6-(4-methoxyphenyl)-1,3,5-hexatrienyl]-1-methyl-, (E,E,E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) MF C19 H20 N O . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Ethanol, 2,2'-[[4-[2-(4-pyridinyl)diazeno]phenyl]imino]bisMF C15 H18 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 4-Piperidinol MF C5 H11 N O C CM

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[2,5-dimethyl-4-(1-piperidinyl)phenyl]methylene]MF C17 H19 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 4-[2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsily]]oxy]ethyl]amino]phenyl]diazenyl]-1-[[4-(dichloroidoxilyl)phenyl]methyl]-, iodide (1:1)

MF C34 H52 C12 I N4 O2 Si3 . I

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

—cı

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 5(4H)-Isoxazolone, 3-phenyl-4-[[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thienyl]methylene]-MF C25 H22 N2 O2 S2

L21 214 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Pyridinium, 1-methyl-4-[2-[4-(1-pyrrolidinyl)phenyl]ethenyl]-, (E)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI)

MF C18 H21 N2 . C7 H7 O3 S

CM 1

Double bond geometry as shown.

L21 214 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzenamine, N,N-dimethyl-4-[2-(2-pyridinyl)ethenyl]-NF c15 H16 W2 C COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 121 and Propanedinitrile 40891 PROPANEDINITRILE

L22 21 L21 AND PROPANEDINITRILE

=> s 121 and dicyanomethylene 5559 DICYANOMETHYLENE

L23 5 L21 AND DICYANOMETHYLENE

=> s 122 or 123

L24 25 L22 OR L23

=> d scan 1-

'1-' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]MF C28 H37 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQID - Same as SQIDE, but 3-letter amino acid codes are used
SQB - Frotein sequence data, includes RN
SQB3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Frotein sequence name information, includes RN

EPROP - Table of experimental properties PPROP - Table of predicted properties PROP - EPROP, ETAG, PPROP

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data
IFC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IFC, and NCL

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available. The MAX format is the same as ALL plus SPEC. The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d scan

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenebutanoic acid, 4-hydroxy-γ-(4-hydroxyphenyl)-γmethyl-, 3-[4-[2-cyano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1(4H)-pyridinyl]propyl ester

C37 H32 N4 O4
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Proparedintrile, 2-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]-MF C11  $49~\rm N3$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]ethylidene]-2,5-cyclohexadien-1-ylidene]-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]ethenyl]phenyl]MF C26 H23 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Proparedinitrile, [[5-[2-[4-[bis(butylphenyl]amino]phenyl]ethenyl]-2thienyl](2, 3, 5, 6-tetrafluoro-4-pyridinyl)methylene]- (9CI)
MF C41 H34 F4 N4 S
C1 IDS

2 ( D1-Bu-n )

$$\begin{array}{c} \text{p1} \\ \text{D1-N} \\ \text{CH} = \text{CH} \\ \end{array}$$

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[4-(1-piperidinyl)phenyl]methylene]MF C15 H15 N3
C1 COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]
MF C28 H37 N3

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)MF C9 H7 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3,5-dimethyl-4-(1,3,5-trimethyl-4(1H)pyridinylidene)-2,5-cyclohexadien-1-ylidene)MF C19 H19 N3
C1 CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[[5-[2-[4-(diphenylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]MF C33 H18 F4 N4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-(4-pyridiny1)pheny1]-, ion(1-), sodium (1:1) MF C14 H8 N3 . Na

• Na+

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[5-[2-[4-(dibutylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]MF C29 H26 F4 N4 5.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[2,5-bis(1-methylethyl)-4-(1-piperidinyl)phenyl]methylene]NF C21 H27 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]-

MF C18 H17 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2thieny1]-2-propen-1-ylidene]
NF C21 H19 N3 S2

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Poly[oxycarbonyl-1,3-phenylenecarbonyloxy-1,4-phenylene[4-[3-[4-[2-cyano-2-[4-(dicyanomethyl-lene]-2,5-cyclohexadien-1-ylidene]ethylidene]-1(4H)-pyridinyl]propoxy]-1-methyl-4-oxobutylidene]-1,4-phenylene] (9CI)

GCI PMS

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

PAGE 1-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Proparedinitrile, 2-[[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2thieny1]methylene]MF C19 H17 N3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[[2,5-diethyl-4-(1-piperidinyl)phenyl]methylene]-

C19 H23 N3 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenebutanoic acid, 4-hydroxy-γ-(4-hydroxyphenyl)-γmethyl-, 3-[4-[2-cyano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1 (4B)-pyridinyl]propyl ester, polymer with
1,3-benzenedicarbonyl dichloride (9CI)

MF (G37 H32 N4 O4 . C8 H4 C12 O2)x

CI PMS

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

CM 2

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[[2,5-dimethyl-4-(1-piperidinyl)phenyl]methylene]-

C17 H19 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[5'-(1-piperidiny1)[2,2'-bithiophen]-5y1]methylene]MF C17 H15 N3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-ymethyl-, 3-[4-[2-cyano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1(4H)-pyridinyl]propyl ester, polymer with
1,3,5-benzenetricarbonyl trichloride (9CI)

MF (C37 H32 N4 O4 . C9 H3 C13 O3)x

CI PMS

CM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[5-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]4-phenyl-2(5H)-thiazolylidene]
MF C20 H14 N4 S

L24 25 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Proparedinitrile, [[5-[2-[5-(1-piperidiny1)-2-thienyl]ethenyl]-2-thienyl]thenyl]-2-thienyl]methylene]-, (E,E)- (9CI)
MF C25 H21 N3 S3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

```
=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
     FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
L1
               STRUCTURE UPLOADED
L2
              0 S L1
L3
             14 S L1 FULL
     FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
     FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
     FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN :
                                   172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
           172 SEA L5
L6
L7
             1 S L3 NOT L6
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L9
             1 S OPTOPHORE
L10
             0 S L3 AND L9
L11
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L12
            26 S ELECTRO-OPTIC CHROMOPHORES
L13
             0 S ELECTROPTIC CHROMOPHORES
L14
             27 S ELECTROOPTIC CHROMOPHORES
L15
         11072 S ELECTROOPTIC
L16
            660 S L15 AND CHROMOPHORE
            679 S L12 OR L14 OR L16
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L19
                                  3023 TERMS
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L20
            214 S L20 AND C5N/RF
L21
L22
             21 S L21 AND PROPANEDINITRILE
             5 S L21 AND DICYANOMETHYLENE
L23
             25 S L22 OR L23
L24
=> s 124 not 13
           25 L24 NOT L3
L25
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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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=> d his

L1

(FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 L4 11 S L3

FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010

FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5 TRA L4 1- RN : 172 TERMS

FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 L6 172 SEA L5

L7 1 S L3 NOT L6

FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 L8 0 S OTOPHORE

```
1 S OPTOPHORE
L9
L10
             0 S L3 AND L9
L11
             12 S L4 OR L9
L12
             26 S ELECTRO-OPTIC CHROMOPHORES
             0 S ELECTROPTIC CHROMOPHORES
L13
L14
             27 S ELECTROOPTIC CHROMOPHORES
L15
          11072 S ELECTROOPTIC
L16
            660 S L15 AND CHROMOPHORE
L17
            679 S L12 OR L14 OR L16
     FILE 'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010
         269403 S C6N/RF
L18
     FILE 'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010
L19
                TRA L17 1- RN :
                                    3023 TERMS
     FILE 'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010
L20
           3023 SEA L19
            214 S L20 AND C5N/RF
L21
             21 S L21 AND PROPANEDINITRILE
L22
              5 S L21 AND DICYANOMETHYLENE
L23
L24
             25 S L22 OR L23
L25
             25 S L24 NOT L3
     FILE 'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010
L26
             99 S L25
     FILE 'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010
```

FILE 'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010

=> analyze 125 ENTER ANSWER NUMBER OR RANGE (1-):1-ENTER DISPLAY CODE (CHEM) OR ?:end

# => help sfields

The searchable fields in the REGISTRY File for general terms, nomenclature-based terms, terms derived from molecular formulas, and property data terms are listed below. If you do not specify a field, your term will be searched in the Basic Index, which contains all name segments, collective index codes, and molecular formula fragments.

CAS Registry Numbers may also be entered without a field code. The system will automatically append /RN to the Registry Numbers before searching them. Registry Numbers containing truncation or character masking must be searched in the /RN field.

Both left and right truncation (SLART) may be used in the /CNS, /NTE, and /ENTE search fields in the REGISTRY File. A term with left truncation must contain at least four characters, for example, S ?CYAN?/CNS. A term with left truncation will retrieve only terms that have at least one alphabetic character, for example, S ?1040/CNS will retrieve C1040/CNS but not 21040/CNS or 1040/CNS.

Numeric fields may be searched as single point values, ranges, or with numeric operators, e.g., 12/S, 200-250/FW, NC >= 3.

Material Composition (MAC) may be searched with both text terms for components and numeric terms for composition. For further information, enter HELP MAC at an arrow prompt (=>).

FIELD NAME	FIELD QUA	ALIFIER
Basic Index CAS Registry Number Locator CAS Registry Number Class Identifier Component Registry Number Definition Editor Note	/BI (or r /LC /RN /CI /CRN /DEF /ENTE	none)
Entry Date Field Availability File Segment Number of References in the CA File	/ED /FA /FS /REF.CA	(numeric)
Number of References in the CA File for non-specific derivatives Number of References in the CAplus File		(numeric)
Polymer Class Term Polymer Class Term Count Source of Registration	/PCT	(numeric)
Update Date  Nomenclature Fields	/UP	(numeric)
Chemical Name Chemical Name Segment Heading Parent Index Name Segment - Heading Parent Index Name Segment - Non-Heading Parent Other Name Segment	/CN /CNS /HP /INS.HP /INS.NHP /ONS	
Molecular Formula Fields		
Atom Count Element Count Element Count for Substance Element Formula	/ATC /ELC /ELC.SUB /ELF	
Element Ratio, xx (xx = CH, CN, CO, HC, HN, HO, NC, NH, NO, OC, OH, ON)	/ELR.xx	(numeric)
Element Symbol Element Symbol for Multicomponent Formula Formula Weight	/ELS.MCF /FW	(numeric)
Material Composition Molecular Formula Number of Components	/MAC /MF /NC	(mixed) (numeric)
		•

Periodic Group	/PG
Relative Composition	/RC
Specific Element Counts	/CU, /NI, etc.(numeric)

The Element Formula (ELF) field requires spaces between the elements in the formula, e.g., => S C H N O/ELF. The Molecular Formula (MF) field may be entered with or without spaces. Formula fragments searched in the Basic Index must be entered without spaces.

CAplus Document Type and	
Super Roles Search Fields	Search Field
Document type	/DT.CA
Super roles for specific substances	/RL
Super roles for non-specific derivatives	/RLD
Super roles for specific substances and non-specific derivatives	/RLS
Super roles for specific substances from patents	/RL.P
Super roles for non-specific derivatives from patents	/RLD.P
Super roles for specific substances and non-specific derivatives	/RLS.P
from patents	
Super roles for specific substances	/RL.NP
from non-patent documents	
Super roles for non-specific	/RLD.NP
derivatives from non-patent documents	
Super roles for specific substances	/RLS.NP
and non-specific derivatives	
from non-patent documents	

REGISTRY contains property data and related information in the following search fields. Unless indicated otherwise in footnote (1), property search fields may be searched using numeric operators or ranges.

Field Name	Search Field	Default Unit
Bioconcentration Factor	/BCF	none
Bioconcentration Factor pH	/BCF.PH	none
Bioconcentration Factor Temp.	/BCF.T	deg C
Boiling Point	/BP	deg C
Boiling Point Pressure	/BP.P	Torr
Density	/DEN	g/cm**3
Density Pressure	/DEN.P	Torr
Density Temperature	/DEN.T	deg C
Electric Conductance	/ECON	Siemens
Electric Conductance Temperature	/ECON.T	deg C
Electric Conductivity	/ECND	S/cm
Electric Conductivity Temperature	/ECND.T	deg C

Electric Resistance	/ERES	ohm
Electric Resistance Temperature	/ERES.T	deg C
Electric Resistivity	/EREST	ohm*cm
Electric Resistivity Temperature	/EREST.T	deg C
Enthalpy of Vaporization	/HVAP	kJ/mol
Enthalpy of Vaporization Pressure	/HVAP.P	Torr
	/EPROPS	
Experimental Properties (1)		none
Experimental Property Tags (2)	/ETAG	none
Flash Point	/FP	deg C
Freely Rotatable Bonds	/FRB	none
Glass Transition Temperature	/TG	deg C
Hydrogen Acceptors	/HAC	none
Hydrogen Donors	/HD	none
Hydrogen Donor/Acceptor Sum	/HDAS	none
Koc (Organic Carbon Adsorption Coeff.	/KOC	none
Koc pH	/KOC.PH	none
Koc Temperature	/KOC.T	deg C
rod lemberatare	/LOGD	none
	· .	
LogD pH	/LOGD.PH	none
LogD Temperature	/LOGD.T	none
LogP	/LOGP	none
LogP Temperature	/LOGP.T	deg C
Mass Intrinsic Solubility	/ISLB.MASS	g/L
Mass Solubility	/SLB.MASS	g/L
Mass Solubility pH	/SLB.PH	none
Magnetic Moment	/MM	muB
Magnetic Moment Temperature	/MM.T	K
Median Lethal Dose	/LD50	mg/kg
Median Lethal Dose Organism	/LD50.ORGN	none
Median Lethal Dose Route of Administration	/LD50.RTE	none
Melting Point	/MP	deg C
Melting Point Pressure	/MP.P	Torr
Melting Point Solvent	/MP.SOL	none
Molar Intrinsic Solubility	/ISLB.MOL	mol/L
Molar Solubility	/SLB.MOL	mol/L
Molar Solubility pH	/SLB.PH	mol/L
Molar Volume	/MVOL	cm**3/mol
	•	
Molar Volume Temperature	/MVOL.T	deg C
Molar Volume Pressure	/MVOL.P	Torr
Molecular Weight	/MW	none
Optical Rotatory Power	/ORP	deg
Optical Rotatory Power Concentration	/ORP.C	g/100mL
Optical Rotatory Power Temperature	/ORP.T	deg C
Optical Rotatory Power Pathlength	/ORP.LEN	dm
Optical Rotatory Power Solvent	/ORP.SOL	none
Optical Rotatory Power Wavelength	/ORP.W	nm
pKa	/PKA	none
pKa Temperature	/PKA.T	deg C
pKa Type	/PKA.TYP	none
Polar Surface Area	/PSA	A**2
rorar barraco inca		gstrom**2)
Property Note (1)	/PNT	none z,
Property Source (1)	/PSO	none
	/PTYP	
Property Type (1)  Peference Accession Number in CA (1)		none
Reference Accession Number in CA (1)	/RAN.CA	none

Refractive Index	/RI	none
Refractive Index Temperature	/RI.T	deg C
Refractive Index Wavelength	/RI.W	nm
Spectra (1)	/SPEC	none
Tensile Strength	/TS	MPa
Tensile Strength Temperature	/TS.T	deg C
Uncertainty Range	/UR	none
Vapor Pressure	/VP	Torr
Vapor Pressure Temperature	/VP.T	deg C

- (1) Field containing text terms which are not searchable with numeric operators or ranges.
- (2) For a list of the tagged properties, refer to REGISTRY: Tagged Experimental Properties at:

www.cas.org/support/stngen/stndoc/properties.html

For information on the sources and definitions of properties, refer to Property Searching in REGISTRY:

www.cas.org/support/stngen/stndoc/properties.html

Enter HELP ROLES at an arrow prompt in the file for a list of CAplus super roles that are searchable in REGISTRY.

Additional information on search or display fields is available in the following messages:

```
HELP SRINGS - list of ring data search fields
HELP SSQ - list of sequence search fields
HELP DFIELDS - list of display field codes
```

```
=> s 125 and 5<=ref.caplus
1484320 5<=REF.CAPLUS
L27 6 L25 AND 5<=REF.CAPLUS
```

=> file caplus
FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 7 Jun 2010 VOL 152 ISS 24

FILE LAST UPDATED: 6 Jun 2010 (20100606/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 127 L29 90 L27 => s 128

L30 13 L28

=> file reg FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4 DICTIONARY FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d his

(FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010

L1 L2 L3	STRUCTURE UPLOADED 0 S L1 14 S L1 FULL
L4	FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 11 S L3
	FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
L5	FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 TRA L4 1- RN: 172 TERMS
L6 L7	FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 172 SEA L5 1 S L3 NOT L6
L8 L9 L10 L11 L12 L13 L14 L15 L16	FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010  0 S OTOPHORE 1 S OPTOPHORE 0 S L3 AND L9 12 S L4 OR L9 26 S ELECTRO-OPTIC CHROMOPHORES 0 S ELECTROPTIC CHROMOPHORES 27 S ELECTROOPTIC CHROMOPHORES 11072 S ELECTROOPTIC 660 S L15 AND CHROMOPHORE 679 S L12 OR L14 OR L16
L18	FILE 'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010 269403 S C6N/RF
L19	FILE 'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010 TRA L17 1- RN : 3023 TERMS
L20 L21 L22 L23 L24 L25	FILE 'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 214 S L20 AND C5N/RF 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE 25 S L22 OR L23 25 S L24 NOT L3
L26	FILE 'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25
	FILE 'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010
L27 L28	FILE 'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 6 S L25 AND 5<=REF.CAPLUS 19 S L25 NOT L27
L29 L30	FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28

FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010

=> d scan 127

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[4-(1-piperidinyl)phenyl]methylene]MF C15 H15 N3
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[[5'-(1-piperidiny1)[2,2'-bithiophen]-5-yl]methylene]MF C17 H15 N3 S2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]-MF C11 H9 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[[5-[2-[4-(diphenylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]
MF C33 H18 F4 N4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]ethylidene]-2(5H)-thienylidene]C1 E21 H24 N4 O2 S
C1 CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L27 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)MF C9 H7 N3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 127 and hydroxyethyl 431333 HYDROXYETHYL L31 1 L27 AND HYDROXYETHYL

=> d scan

L31 1 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(IH)-pyridinylidene]ethylidene]-2(5H)-thienylidene]MF C21 H24 N4 O2 S
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

L28

=> d his (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010) FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 L1 STRUCTURE UPLOADED L2 0 S L1 L3 14 S L1 FULL FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 L411 S L3 FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010 FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5TRA L4 1- RN : 172 TERMS FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 172 SEA L5 L6 L7 1 S L3 NOT L6 FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 L8 0 S OTOPHORE L9 1 S OPTOPHORE L10 0 S L3 AND L9 L11 12 S L4 OR L9 L12 26 S ELECTRO-OPTIC CHROMOPHORES L13 0 S ELECTROPTIC CHROMOPHORES L1427 S ELECTROOPTIC CHROMOPHORES L15 11072 S ELECTROOPTIC L16 660 S L15 AND CHROMOPHORE 679 S L12 OR L14 OR L16 L17 FILE 'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010 L18 269403 S C6N/RF FILE 'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010 TRA L17 1- RN : L19 3023 TERMS FILE 'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 L20 214 S L20 AND C5N/RF L21 L22 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE L23 25 S L22 OR L23 L24 L25 25 S L24 NOT L3 FILE 'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25 L26 FILE 'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010 FILE 'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 L27 6 S L25 AND 5<=REF.CAPLUS

19 S L25 NOT L27

FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010

L29 90 S L27 L30 13 S L28

FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 L31 1 S L27 AND HYDROXYETHYL

=> file caplus FILE 'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 7 Jun 2010 VOL 152 ISS 24

FILE LAST UPDATED: 6 Jun 2010 (20100606/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 131

L32 6 L31

=> d his

(FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010

L4 11 S L3

=> s 132 or 130

	FILE	'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
<b>1</b> 5	FILE	'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 TRA L4 1- RN : 172 TERMS
_6 _7	FILE	'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 172 SEA L5 1 S L3 NOT L6
18 19 110 111 112 113 114 115 116 117		'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010  0 S OTOPHORE  1 S OPTOPHORE  0 S L3 AND L9  12 S L4 OR L9  26 S ELECTRO-OPTIC CHROMOPHORES  0 S ELECTROPTIC CHROMOPHORES  27 S ELECTROOPTIC CHROMOPHORES  11072 S ELECTROOPTIC  660 S L15 AND CHROMOPHORE  679 S L12 OR L14 OR L16
L18		'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010 269403 S C6N/RF
L19	FILE	'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010 TRA L17 1- RN : 3023 TERMS
L20 L21 L22 L23 L24 L25	FILE	'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 214 S L20 AND C5N/RF 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE 25 S L22 OR L23 25 S L24 NOT L3
L26	FILE	'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25
	FILE	'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010
_27 _28	FILE	'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 6 S L25 AND 5<=REF.CAPLUS 19 S L25 NOT L27
L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32	FILE	'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31

L33 19 L32 OR L30

=> d cbib abs hitstr 1-YOU HAVE REQUESTED DATA FROM 19 ANSWERS - CONTINUE? Y/(N):y ANSWER 1 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 1:607268 Document No. 149:319620 Twisted x-Electron System Electrooptic Chromophores. Structural and Electronic Consequences of Relaxing Twist-Inducing Nonbonded Repulsions. Wang, Yiliang;

arelli,
David L.; Facchetti, Antonio; Cariati, Elena; Tordin, Elisa; Ugo, Renato;
Zuccaccia, Cristiano; Macchioni, Alceo; Wegener, Staci L.; Stern,
Charlotte L.; Ratner, Mark A.; Marks, Tobin J. (Department of Chemistry
and the Materials Research Center, Northwestern University, Evanston, IL,
60208-313, USA). Journal of Physical Chemistry C, 112(21), 8005-8015
(English) 2008. CODEN: JPCCCK. ISSN: 1932-7447. CTHER SOURCES: CASREACT

CASREACT

149:31962. Publisher: American Chemical Society.

AB The synthesis, structural and spectroscopic characterization, and nonlinear optical response properties of a "slightly" twisted zwitterionic

4-quinopyran electrooptic chromophore FMC,
2-(4-{1-(2-propylheptyl)-lH-pyridine-4-ylidene]cyclohexa-2,5-dienylidene]malonomitrile, are reported. X-ray diffraction data and d. functional theory (DFT) minimized geometries confirm that deletion of the four o-, o'-, o''-, and o'''-Me groups in the parent chromophore TMC-2,
2-(4-{13,5-dimethyl-1-(2-propylheptyl)-lH-pyridin-4-ylidene]-3,5-dimethylcyclohexa-2,5-dienylidene|malonomitrile, relaxes the arene-arene twist angle from 89,6 to 9.0°. These geometrical changes result in a significantly increased contribution of the quinoidal structure to the mol. ground state of FMC (vs. TMC-2), reduced solvatochromic shifts in

optical spectra, and a diminished elec.-field-induced second-harm (EFTSH) generation derived mol. hyperpolarizability ( $\mu\beta$  = -2340 + 10-48 esu of DFMC, the dendrimer derivative of FMC, vs -24000 + 10-48 esu of TMC-2) in CH2C12 at 1907 nm. Pulsed field gradient spin-echo

-echo
(PGSE) NMR spectroscopy and EFISH indicate that the levels of FMC
aggregation in solution are comparable to those of TMC-2 (monomers and
dimers) in CH2Cl2 solution B3LYP and INDO/S computation of chromophore

mol. structure, aggregation, and hyperpolarizability trends are in good agreement with experiment 1031421-49-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT TT

(Reactant or reagent)

(synthesis, structural and spectroscopic characterization, and nonlinear optical response properties of "slightly" twisted zwitterionic 4-quinopyran electrooptic chromophore)

Propanedinitrile, 2-[4-(4-pyridinyl)phenyl]-, ion(1-), sodium (1:1) (CA INDEX NAME)

L33 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2007:196777 Document No. 146:4234930 Ultralarge hyperpolarizability twisted \*\*-electron system electro-optic chromophores: Synthesis, solid-state and solution-phase structural characteristics, electronic structures, linear and nonlinear optical properties, and computational studies.

Hu; Facchetti, Antonio; Jiang, Hua; Cariati, Elena; Righetto, Stefania; Ugo, Renato; Zuccaccia, Cristiano; Macchioni, Alceo; Stern, Charlotte L.; Liu, Zhifu; Ho, Seng-Tiong; Brown, Eric C.; Ratner, Mark A.; Marks, Tobin J. (Pepartment of Chemistry and the Materials Research Center and Department of Electrical and Computer Engineering, Northwestern University, Evanston, IL, 60208-3113, USA). Journal of the American Chemical Society, 129(11), 3267-3286 (English) 2007. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 146:423493. Publisher: icen

ISSN: 0002-000.

American
Chemical Society.

AB This contribution details the synthesis and chemical/phys.

characterization
of a series of 5 unconventional twisted \( \pi \)-electron system electro-optic
(EO) chromophores. Crystallog. anal. of these twisted intramol. charge-transfer chromophores reveals large ring-ring dihedral twist

Angles

Angl

is (80-89°) and a highly charge-separated zwitterionic structure dominating the ground state. NOE NMR measurements of the twist angle in solution confirm that the solid-state twisting persists essentially unchanged

in solution Optical, IR, and NMR spectroscopic studies in both the solution phase and solid state further substantiate that the solid-state

structural characteristics persist in solution The aggregation of these highly

polar

pyridinium zwitterions is investigated using several exptl. techniques, including concentration-dependent optical and fluorescence spectroscopy

pulsed field gradient spin-echo NMR spectroscopy in combination with solid-state data. These studies reveal clear evidence of the formation of

centrosym, aggregates in concentrated solns, and in the solid state and provide

quant. information on the extent of aggregation. Solution-phase DC elec.-field-induced second-harmonic generation (EFISH) measurements

Unprecedented hyperpolarizabilities (nonresonant  $\mu\beta$  as high as -488 000 + 10-48 esu at 1907 nm). Incorporation of these chromophores into guest-host poled polyvinylphenol films provides very large EO coeffs. (r33) of .apprx.330 pm/V at 1310 nm. The aggregation

structure-property effects on the observed linear/nonlinear optical properties are discussed. High-level computations based on e-averaged complete active space SCF methods provide a new rationale for these exceptional hyperpolarizabilities and demonstrate significant solvation effects on hyperpolarizabilities, in good agreement with experiment \( \text{\text{AS}} \)

this work suggests new paradigms for mol. hyperpolarizabilities and

electro-optics. 866416-39-9P 866416-43-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

L33 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Na +

L33 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

(intermediate; prepn., hyperpolarizability and spectra of twisted
pyridinium-based chromophores)

RN 866416-39-9 CAPLUS

CN Propanedinitrile, 2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl](CA INDEX NAME)

866416-43-5 CAPLUS
Propanedinitrile, 2-[4-[2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]ethenyl]phenyl]- (CA INDEX NAME)

866416-40-2P 866416-41-3P

866416-40-2P 866416-41-3P RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (orange chromophore; preparation, hyperpolarizability and spectra of twisted

twisted
pyridinium-based chromophores)
RN 866416-40-2 CAPLUS
RN Propanedinitrile
2-[3,5-dimethyl-4-[1,3,5-trimethyl-4(1H)-pyridinylidene)2,5-cyclohexadieni-ylidene]- (CA INDEX NAME)

866416-41-3 CAPLUS
Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]- (CA INDEX
NAME)

L33 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

866416-44-6P RL: PRP (Properties); SFN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (purple chromophore; preparation, hyperpolarizability and spectra of

ted
pyridinium-based chromophores)

866416-44-6 CAPLUS
Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)pyridinyldene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]ethylidene]-2,5cyclohexadien-1-ylidene]- (CA INDEX NAME)

$$\begin{array}{c} \text{n-Pr} \\ \text{CH} \\ \text{CH-CH-} \end{array}$$

L33 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

866416-41-3 CAPLUS
Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]- (CA INDEX NAME)

866416-44-6 CAPLUS

Propanedinitrile, 2-[4-[2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]- (CA INDEX NAME)

866416-39-9P 866416-43-5P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(twisted K-electron system chromophore compds. with very large mol. hyperpolarizabilities for use in electrooptical devices)
866416-39-9 CAPLUS
Propanedinitrile, 2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]-(CA INDEX NAME)

L33 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2006:1005693 Document No. 145:3360080 Twisted x-electron system chromophore compounds with very large molecular hyperpolarizabilities and related compositions and devices. Marks, Tobin J.; Kang, Hu

(Northwestern
University, USA). PC
DESIGNATED STATES: W: PCT Int. Appl. Wo 2006102620 A2 20060928, 78 pp. W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW,

BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JF, KE, KG, IM, KN, KF, KR, KZ, LC, LK, LK, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MM, MK, MZ, NA, NG, NI, NO, NZ, CM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA; RN: AT, EE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.

CHG1S2A APPLICATION: WO 2006-US10902 20060324. PRIORITY: US

GT

A chromophore compound of a formula (I) wherein X is selected from NR',

and S; each of R' and R1-R4 is independently selected from linear alkyl, substituted linear alkyl, branched alkyl, substituted branched alkyl, cycloalkyl and substituted cycloalkyl moieties; and Y comprises a substitutent comprising a moiety selected from anionic carbon and heteroatom moieties, and salts, conjugate acids and charge-transfer isomers thereof. These unconventional twisted x-electron system electro-optic chromophores were used in electro-optical devices. Crystallog, anal. of several of these chromophores reveals large -ring

ring-ring
dihedral twist angles and a highly charge-separated zwitterionic

structure in

structure in the ground state, in both solution phase and solid-state.

186416-40-2P 866416-41-3P 866416-44-6P RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PRPP (Preparation); USES (Uses) (twisted #-electron system chromophore compds. with very large mol. hyperpolarizabilities for use in electrooptical devices)

RN 866416-40-2 CAPLUS

CN Propanedinitrile,
2-[3,5-dimethyl-4(1,7,5-trimethyl-4(1H)-pyridinylidene)-2,5-cyclohexadien-1-ylidene]- (CA INDEX NAME)

L33 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

866416-43-5 CAPLUS
Propanedinitrile, 2-[4-[2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]ethenyl]phenyl]- (CA INDEX NAME)

ANSWER 4 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN :854700 Document No. 145:512874 Effects of alkyl subsistents of photosefractive chromophores on electro-optic response. Choi, Chil-Sung; Nguyen, Quoc Vuong; Oh, Jin-Woo; Hwang, Ui-Jung; Kim, Nakjoong (Center

Organic Photorefractive Materials Department of Chemistry, Hanyang University, S. Korea). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 47(2), 994-995 (English) 2006. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Folymer Chemistry.

4-Piperidinobenzylidene-malononitrile derivs. with various alkyl subsistents, such as Me, Et and iso-Pr were synthesized. The effect of alkyl groups attached to chromophore on electro optical properties and response time was studied. As the temperature of the sample was raised,

electro-optic response speeded up. Also, bulky alkyl substituents in chromophore provide some free volume to facilitate the rotational

chromophore provide some free volume to facilitate the rotational mobility, characteristic formula on temperature and shape of chromophores.

IT 915021-99-7 915022-00-3 915022-01-4 RL DEV (Device component use); MOA (Modifier or additive use); PRP (Properties); USES (Uses) (dopant; effects of alkyl subsistents of photorefractive chromophores on electro-optic response)

RN 915021-99-7 CAPLUS
CN Propanedinitrile, 2-[[2,5-dimethyl-4-(1-piperidinyl)phenyl]methylene]-(CA INDEX NAME)

RN

915022-00-3 CAPLUS Propanedinitrile, 2-[[2,5-diethyl-4-(1-piperidinyl)phenyl]methylene]-(CA

INDEX NAME)

L33 ANSMER 5 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
2006:610326 Document No. 145:250751 Effect of conjugation path length on
quadratic nonlinear optical properties of monomer and aggregates of
zwitterionic merocyanine dyes. Ray, Paresh C.; Bonifassi, P.;
Leszczynski, J. (Department of Chemistry, Jackson State University,
Jackson, MS. 39217, USA). Journal of Physical Chemistry A, 110(28),
8963-8969 (English) 2006. CODEN: JPCAFH. ISSN: 1089-5639. Publisher:
American Chemical Society.
AB We present a quantum-chemical anal. of the conjugation path length
effect on

AB we present a guaranteeffect on

first hyperpolarizabilities of a series of 3 zwitterionic merocyanine

whose synthesis has been reported earlier. The effect of the conjugation path lengths is evaluated to demonstrate the engineering guidelines for enhancing mol. optical nonlinearity. The first hyperpolarizabilities are calculated for extended conjugated monomer and H and J type aggregates of merocyanine dyes, to provide insight into the intermol. interactions and the relationship between structural and collective nonlinear optical properties. The mol. geometries for monomers are obtained via B3LYP6-31G(d,p) level optimization including the SCRF/FCM approach, and the dynamic nonlinear optical (NLO) properties for monomer and aggregates are calculated with the ZINDO/CV method, including solvent effects. It

found that the chain length dependence of the first nonlinearity peaks at n = 6 and then it starts changing slowly for monomer and aggregates of zwitterionic merocyanine dyes. It is concluded that an excellent NL response in solution might vanish when the active chromophore forms

aggregates. The importance of our results on the design of electrooptic materials has been discussed. 905990-23-0 higher H

RL: PRP (Properties); TEM (Technical or engineered material use); USES

(Uses)

(Uses)
 (dye; effect of conjugation path length on NLO properties of monomer
 and aggregates of zwitterionic merocyanine dyes)
930590-23-0 CAPLUS
Propanedinitrile, 2-[5-[2-(1-methyl-4(1H)-pyridinylidene)ethylidene]-4phenyl-2(5H)-thiazolylidene]- (CA INDEX NAME)

(Continued)

L33 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN RN 915022-01-4 CAPLUS CN Proparedintrile, 2-[[2,5-bis(1-methylethyl)-4-(1-piperidinyl)phenyl]methylene]- (CA INDEX NAME)

33 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
106:532360 Document No. 145:220599 Electro-optics poled sol-gel materials
doped with heterocycle push-pull chromophores. Della Giustina, Gioia;
Brusatin, Giovanna; Guglielmi, Massimo; Dispenza, Massimiliano; Fiorello,
Anna Maria; Varasi, Mauro; Casalboni, Mauro; Quatela, Alessia; De

Matteis,
Fabio; Giorgetti, Emilia; Margheri, Giancarlo; Innocenzi, Plinio;
Abbotto,
Alessandro; Beverina, Luca; Pagani, Giorgio A. (Dipartimento di

Alessandro; Beverina, Luca; Pagani, Giorgio A. (Dipartimento di Ingegneria Meccanica, Settore Materiali and INS, Padua, 35131, Italy). Materials Science & Engineering, C: Biomimetic and Supramolecular Systems, 26(5-7), 979-982 (English) 2006. CODEN: MSCEEE. ISSN: 0928-4931. Publisher: Elsevier B.V.

AB Hybrid organic-inorg. materials doped with zwitterionic push-pull chromophores with high hyperpolarizability were synthesized via sol-gel, based on glycidoxypropylethyldimethoxysilane (GPTMS) and glycidoxypropylethyldimethoxysilane (GPTMS) and glycidoxypropylmethyldimethoxysilane (GPTMS). Homogeneous films doped with chromophores, were obtained using N-hydroxyethylcarbazole as a phys. spacer avoiding dye aggregation. The waveguiding properties of the spin-coated doped films elec. poled in N2 atmosphere showing 2nd harmonic generation measurements, were preliminarily measured by m-line spectroscopy before and after poling; the feasibility of channel waveguiding structures was demonstrated.

IT 468721-53-1

RI: DEV (Device component use); MOA (Modifier or additive use); USES (USES)

(Uses)

(Uses)
(electrooptic poled sol-gel materials doped with)
468721-53-1 CAPLUS
Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]-t(2H)-thienylidene]- (CA INDEX NAME)

ANSWER 7 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 5:1007743 Document No. 143:3758400 Synthesis and unprecedented electro-optic response properties of twisted r-system chromophores. Kang, Hu, Facchetti, Antonio, Jiang, Hua, Zhu, Peiwang; Marks, Tobin J. (Department of Chemistry and the Materials Research Center, Northwestern University, Evanston, II., 60208-3113, USA). Materials Research Society Symposium Proceedings, 866(Rare-Earth Doping for Optoelectronic Applications), 131-136 (Emglish) 2005. CODEN: MRSDH. ISSN: 0272-9172. OTHER SOURCES: CASREACT 143:375840. Publisher: Materials Research Society.

OTHER SOURCES: CASREACT 143:375440. Publisher: Materials Research Society. Symposium proceedings. A series of unconventional twisted intramol. charge-transfer (TICT) chromophores was designed and synthesized. Chromophores exhibit ultra-large first hyperpolarizabilities. The structural characteristic that promotes this unusual nonlinear optic response is a stereochem. enforced reduction of the D-π-A conjugation.

response is a stereochem, entoreed reduction of the D-AA conjugation enforces zwitterionic behavior in the ground state and provides a low-energy, large-oscillator strength intramol, excitation feature. The consequence is that mols, with relatively small nos, of  $\pi$ -electrons exhibit responses far larger than those of traditional planar  $\pi$ -conjugated chromophores. At 1907 nm, non-resonant  $\mu\beta$  values as high as -466,000 + 10-48 esu are observed 866416-39-9P 866416-43-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (quaternization/deprotonation; synthesis and unprecedented electro-optic response properties of twisted intramol. charge-transfer  $\pi$ -system chromophores) 866416-39-9 CAPLUS Propanedinitrile, 2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]-(CA INDEX NAME)

RN

866416-43-5 CAPLUS
Propanedinitrile, 2-[4-[2-[4-(3,5-dimethyl-4-pyridinyl)-3,5-dimethylphenyl]ethenyl]phenyl]- (CA INDEX NAME)

L33 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN

L33 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Continued)

866416-41-3P 866416-44-6P
RL: MOA (Modifier or additive use); PRP (Properties); SFN (Synthetic preparation); PREP (Preparation); USES (Uses)
(synthesis and unpracedented electro-optic response properties of twisted intramol. charge-transfer x-system chromophores)

866416-41-3 CAPLUS
Propanedinitrile, 2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]- (CA INDEX NAME)

(CA INDEX

866416-44-6 CAPLUS
Propanedinitrile, 2-[4-[2-[4-[3,5-dimethyl-1-(2-propylheptyl)-4(1H)-pyridinylidene]-3,5-dimethyl-2,5-cyclohexadien-1-ylidene]-thylidene]-2,5-cyclohexadien-1-ylidene]- (CA INDEX NAME)

IT 866416-40-2P

ANSWER 8 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 180530 Document No. 142:3369710 A New Approach to Highly Electrooptically Active Materials Using Cross-Linkable, Hyperbranched Chromophore-Containing Oligomers as a Macromo

Song, Naiheng; Gao, Jian Ping; Sun, Xun; Wang, Xiaomei; Yu, Guomin; Wang, Zhi Yuan (Department of Chemistry, Carleton University, Ottawa, ON, KIS 586, Can.). Journal of the American Chemical Society, 127(7), 2060-2061 (English) 2005. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES:

(English) 2005. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES:
CASREACT
142:336971. Publisher: American Chemical Society.

A A new, practical approach to a variety of highly electrooptically active polymers for device development is described. It involves the use of a new thermally cross-linkable, hyperbranched oligomer containing nonlinear optical (NLO) chromophores as a macromol. dopant in a common host

polymer.

optical (NLO) enromophores as a macromol. dopant in a common host
mer.

A series of NLO polymeric blends were readily formulated and showed large
and stable electrooptic (EO) coeffs. (up to 65 pm/V). In comparison with
previously studied linear NLO polyimides and guest-host polymers doped
with mol. chromophores and even linear NLO analogous oligomers, this new
approach offers clear advantages for device development in terms of
improved poling efficiency, larger EO coeffs., good temporal stability,
and versatile material formulation.
848599-33-TDP, reaction products with aminobenzocyclobutenone
848599-34-BP 848599-35-9P
RL: PRP (Properties)) SPN (Synthetic preparation); PREP (Preparation)
(crosslinkable hyperbranched chromophore-containing oligoesters as
macromol. dopants for highly electrooptically active materials)
848599-33-7 CAPLUS
Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-y-methyl-,

848599-33-7 CAPLUS
Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-y-methyl-,
3-[4-[2-cyano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1(4H)-pyridinyl]propyl ester, polymer with
1,3,5-benzenetricarbonyl trichloride (9CI) (CA INDEX NAME)

CM 1

CRN 848599-30-4 CMF C37 H32 N4 O4

CRN 4422-95-1

L33 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN CMF C9 H3 C13 O3 (Continued)

848599-34-8 CAPLUS
Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-y-methyl-,
3-[4-[2-cyano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1ylidene]ethylidene]-1(4M)-pyridinyl]propyl ester, polymer with
1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CRN 848599-30-4 CMF C37 H32 N4 O4

CM

CRN 99-63-8 CMF C8 H4 C12 O2

L33 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(monomer; crosslinkable hyperbranched chromophore-contg. oligoesters

macromol. dopants for highly electrooptically active materials) 848599-30-4 CAPLUS Benzenebutanoic acid, 4-hydroxy-\(\gamma\)-(4-hydroxyphenyl)-\(\gamma\)-methyl-, 3-[4-[2-yano-2-[4-(dicyanomethylene)-2,5-cyclohexadien-1-ylidene]-thylidene]-1(4H)-pyridinyl]propyl ester (CA INDEX NAME)

L33 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 848599-35-9 CAPLUS

CN
Poly[oxycarbonyl-1,3-phenylenecarbonyloxy-1,4-phenylene[4-[3-[4-[2-cyano-2[4-(dicyanomethylene]-2,5-cyclohexadien-1-ylidene]ethylidene]-1(4H)pyridinyl]propoxy]-1-methyl-4-oxobutylidene]-1,4-phenylene] (9CI) (CA
INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 848599-30-4P

L33 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2004;977311 Document No. 142:143476 Foled sol-gel materials doped with heterocycle-based push-pull chromophores with second-order optical non-linearity. Brusatin, Giovanna; Innocenzi, Plinio; Guglielmi, Massimo; Abbotto, Alessandro; Beverina, Luca; Pagani, Giorgio A.; Casalboni,

Abbotto, Alessandro; Beverina, Luca; Pagani, Giorgio A.; Casalboni,
Mauro;
Sarcinelli, Felice (Dipartimento di Ingegneria Meccanica, Settore
Materiali, Universita di Padova, Padua, 35131, Italy). Journal of
Non-Crystalline Solids, 345346, 575-579 (English) 2004. CODEN: UNCSBJ.
ISSN: 0022-3093. Publisher: Elsevier B.V..

AB In this work, a previously studied system of a hybrid sol-gel material
doped with a push pull chromophore is optimized by co-doping the matrix
with carbazole functionalized units, and achieving enhanced second order
NLO properties. The microstructure modifications of the hybrid sol-gel
matrix have been investigated during the thermal treatment and the poling
procedure, together with the stability of the dopants. The thermal
treatment performed during the poling process dets. the carbazole units
degradation while the chromophore mols. remain unaltered and their
absorbance

degradation while the chromophore mole. Lemman. degradation while the chromophore mole. Lemman. degradation cefeatures are strongly modified.

IT 468721-53-1P
RL: MOA (Modifier or additive use); FNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); USES (Uses) (chromophore; poled sol-gel materials doped with heterocycle-based push-pull chromophores with second-order optical non-linearity)

RN 468721-53-1 CAPLUS
CN Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]ethylidene]-2(5H)-thienylidene]- (CA INDEX NAME)

ANSWER 10 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
4:906026 Document No. 141:386133 Hybrid organic-inorganic material with
nonlinear optical response based on organic chromophores and process for
the preparation thereof. Sarcinelli, Felice; Abbotto, Alessandro;
Beverina, Luca; Fagani, Glorgio; Brusatin, Glovanna; Innocenzi, Plinio;
Casalboni, Mauro (Universita'Degli Studi di Milano-Bicocca, Ttaly;
Chinelli, Maria Giovanna) - PCT Int. Appl. Wo 2004092820 Al 20041028, 23
pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR,
BM, BY, BZ, CA, CH, CN, CO, CC, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES,
FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ,
LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MM, MM, MM, MX, MX, NA, NI, NN,
NN, CM, PG, PH, PL, FT, RO, RU, SC, SD, SE, SC, SK, SL, SY, TJ, TM, TN,
TT, TZ, UA, UG, US, UZ, VC, VN, VU, 2A, CM, VM, FW: AT, BE, BF, BJ,
CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC,
MM, MR, NE, NL, PT, SE, SN, TD, TO, TR. (English). CODEN PIXXD2.
APPLICATION: WO 2004-EP3594 20040405. PRIORITY: TI 2003-PD80 20030418.
Hybrid organic-inorg. nonlinear optical materials comprising
ss-linked
matrix hosting ≥1 organic chromophore which may be dipole-oriented
using elect. fields are described which include an effective amount of
carbazole derivs. compds. having a Cl-18 (un)branched alkyl chain with
≥1 hydroxyl group bonded to the N and substituents independently
selected from H, lower alkyl, and aryl groups bonded to the ring carbons.
Methods for preparing the materials are described which entail providing
cross linked matrix wherein an organic chromophore is hosted in which the

cross linked matrix wherein an organic chromophore is hosted in which the carbazole derivs. are provided in the matrix. Sol-gel processing may be used to provide the materials. Electrooptical modulators employing the materials are also described. 468721-53-1
RL: DEV (Device component use); MOA (Modifier or additive use); USES

(Uses)

(hybrid organic-inorg. materials with nonlinear optical response based on

organic chromophores and their preparation and use)
468721-53-1 CAPLUS
Propanedinitrile, 2-(5-[2-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]ethylidene]-2(5H)-thienylidene]- (CA INDEX NAME)

L33 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
2002:815193 Document No. 138:392551 Entrapping of Push-Pull Zwitterionic
Chromophores in Hybrid Matrices for Photonic Applications. Innocenzi,
Plinic; Brusatin, Giovanna; Abbotto, Alessandro; Beverina, Luca; Pagani
Giorgio A.; Casalboni, Mauro; Sarcinelli, Felice; Pizzoferrato, Roberto
(Dipartimento di Ingegneria Meccanica, Universita di Padova, Padua,

I, Italy). Journal of Sol-Gel Science and Technology, 26(1/2/3), 967-970 (English) 2003. CODEN: JSGTEC. ISSN: 0928-0707. Publisher: Kluwer Academic Publishers.

A new class of heterocycle-based push-pull chromophores showing enhanced nonlinear properties characterized by an aromatic and highly zwitterionic ground state and a quinoid/neutral excited state have been synthesized to be incorporated in sol-gel hybrid systems. This class of compds. shows very large 1st mol. hyperpolarizabilities (Bn £27000 + 10-48 esu) and is a promising candidate for photonic applications where large 2nd order nonlinearities are required. In spite of their

very large hyperpolarizability and chemical and thermal stability, these chromophores are decomposed in presence of light and  $\circ$  (photobleaching)

are sensitive to acidic environments due to the carbanionic nature of the donor moiety. A hybrid matrix, based on N-[(3-trimethoxysily1)propyl]ethylenediamine and 3-qlycidoxypropyltrimethoxysilane, was specifically designed to allow the incorporation of such zwitterionic compds. assuring at the same time a good temporal stability of the optical properties. Amine functionalization was found very effective in reducing the photobleaching by acting on these chromophores via the singlet 0. Second harmonic generation was observed on poled films, and an order parameter,  $\Phi$ , of 0.17 was estimated The nonlinear coefficient deff of the samples was estimated at thus estimated at

estimated at a value 2 times larger than for dll of quartz that, from literature data, is .apprx.0.335 pm/V. 468721-53-1

TT

400/21-33-1 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES

(Uses)

(coses)

(entrapping of push-pull zwitterionic chromophores in hybrid matrixes for photonic applications)
468721-53-1 CAPLUS
Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]ethylidene]-2(5H)-thienylidene]- (CA INDEX NAME)

L33 ANSMER 11 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2004:43724 Document No. 141:92821 Hybrid organic-inorganic materials containing poled zwitterionic push-pull chromophores. Brusatin, Giovanna:

nna; Innocenzi, Plinio; Abbotto, Alessandro; Beverina, Luca; Pagani, Giorgio A.; Casalboni, Mauro; Sarcinelli, Felice; Pizzoferrato, Roberto (Dipartimento di Ingegneria Meccanica, Universita di Padova, Padua, 35131.

Italv). Journal of the European Ceramic Society, 24(6), 1853-1856 1) 2004. CODEN: JECSER. ISSN: 0955-2219. Publisher: Elsevier

(English) 2004. CODEN: JECSER. ISSN: 0955-2219. Publisher: Elsevier Science Ltd..

AB Dihydroxy-functionalized zwitterionic push-pull chromophores have been introduced in 3-qlycidoxypropyltrimethoxysilane, tetraethylorthosilicate and N-[(3-trimethoxysily1)propyl]ethylenediamine derived hybrid materials.

Hybrid films have been deposited as thick layers via spin-coating. The amine groups introduced with the organically modified alkoxide bearing amine functionalities have an effective scavenger effect of the dye photobleaching. The addition, during the synthesis of the precursor sol, of

sol, of
N-hydroxyl carbazole has allowed to reach up to 20% of chromophore
concentration
avoiding the formation of aggregates within the matrix. The nonlinear
optical properties of the material, after poling, have a good temporal
stability, with retention of .apprx.70% of the initial signal value,

several months, providing a d33 value of .apprx.50+70 pm V-1 at the wavelength of 1.064 µm. 468721-53-1 RL: PRP (Properties); TEM (Technical or engineered material use); USES

(BisOH.PETCN,zwitterionic chromophore, composites with ceramer matrix; preparation and properties of hybrid organic-inorg. materials containing poled

ining poled
 zwitterionic push-pull chromophores as nonlinear optical materials)
468721-53-1 CAPLUS
Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)pyridinylidene]ethylidene]-2(5H)-thienylidene]- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CN} \\ \text{CH} \\$$

L33 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
2002:582770 Document No. 137:301479 Incorporation of zwitterionic push-pull
chromophores into hybrid organic-inorganic matrixes. Innocenzi, Plinic;
Miorin, Enrico; Brusatin, Giovanna; Abbotto, Alessandro; Beverina, Luca;
Pagani, Giorgio A.; Casalboni, Mauro; Sarcinelli, Felice; Pizzoferrato,
Roberto (Department of Mechanical Engineering, Materials Section,
University of Padova, Padua, 1-35131, Italy). Chemistry of Materials,
14(9), 3758-3766 (English) 2002. CODEN: CMAREX. ISSN: 0897-4786.
Publisher: American Chemical Society.

AB Dihydroxy-functionalized zwitterionic push-pull chromophores were
synthesized and incorporated into 3-glycidoxypropyltrimethoxysilane- and
N-[(3-trimethoxysily))propyljethylendiamine-derived hybrid materials.
The functionalization allowed the dye to form covalent bonds to the
matrix

network, reaching up to 5% molar concentration without aggregation. The

hybrid material was also specifically designed to reduce photobleaching

the dye and to avoid the protonation of the carbanionic species that occurs in acidic media. The host material exhibits very good

film-forming

properties, and thick highly transparent doped layers can be fabricated
via dip-coating. Upon incorporation into the matrix, the dye exhibits a
reduction of photobleaching due to the scavenger effect of the amine

groups.

The strong neg. solvatochromism exhibited by this class of chromophores

The strong neg. solvatochromism exhibited by this class of chromophores. The strong neg. solvatochronism exhibited by this class of chromophore was used to probe the phys.-chemical environment within the pores. Dye-functionalized hybrid sol-gel materials were submitted to poling expts., and the second harmonic signal was measured. Good temporal stability of the NLO materials (retention of .apprx.85% of the initial signal value) was recorded after 3 mo, providing a d33 value equal to 0.66

pm/V. This system represents one of the few examples of the successful incorporation of zwitterionic push-pull chromophores in sol-gel pm/V.

materials. IT 468721-53-1P

468721-53-1P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); PRCC (Process) (incorporation of zwitterionic push-pull chromophores into hybrid organic-inorg, matrixes)
468721-53-1 CAPLUS
Propanedinitrile, 2-[5-[2-[1-[3-[bis(2-hydroxyethyl)amino]propyl]-4(1H)-pyridinylidene]ethylidene]-2(5H)-thienylidene]- (CA INDEX NAME)

L33 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2000:819816 Document No. 134:154859 Design and synthesis of highly efficient

nonlinear optical chromophores. Wu, Xiaoming; Jen, Alex K.-Y.

(Department of Chemistry, Northeastern University, Boston, MA, 02115, USA). Materials

rials
Research Society Symposium Proceedings, 598 (Electrical, Optical, and Magnetic Properties of Organic Solid-State Materials V),
BBI1.45/1-BBI1.45/5 (English) 2000. CODEN (MRSPDH. ISSN: 0272-9172.
Publisher: Materials Research Society.
Two series of highly hyperpolarizable nonlinear optical (NLO) chromophores, containing perfluoroaryl dicyanovinyl and Ph tetracyanobutadienyl acceptors, have been designed and synthesized.

These
chromophores show good thermal and chemical stability. The 3D
conformational
structures, confirmed by computational modeling, enhance polymer matrix
compatibility and decrease optical loss of the polymer films. The
guest-host polymers of the chromophores show large electro-optical
activities.

IT 302965-26-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(design and synthesis of highly efficient nonlinear optical
chromophores)
RN 302965-26-0 CAPLUS
CN Proparadinitrile, 2-[[5-[2-[4-(dibutylamino)phenyl]ethenyl]-2thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene] - (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH} & \text{CH} & \text{CH} & \text{CH} \\ \hline \end{array}$$

L33 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

$$2\Bigg[ \bigcirc \Bigg]$$

2 ( D1-Bu-n )

L33 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 2000:414740 Document No. 133:322367 Design and synthesis of highly efficient

chromophores and polymers for electro-optic applications. Jen, Alex

chromophores and polymers for electro-optic applications. Jen, Alex , Ma, Hong; Wu, Xiaoming; Wu, Jianyao; Liu, Sen; Herguth, Fetra; Marder, Seth R.; Shu, Ching-Fong; Dalton, Larry R. (Department of Chemistry, Northeastern University, Boston, MA, 02115, USA). MCIC SET, Section B: Nonlinear Optics, 2(2(1-4), 9-14 (English 1999. CODEN: MCLOEB. ISSN: 1058-7268. Publisher: Gordon & Breach Science Publishers.
A series of highly efficient, chemical and thermally stable (Td ≤ 390°) nonlinear optical chromophores were developed by using a 2-tetrafluoropyridinyl-dicyanovinyl group as the electron acceptor for a series of dialkyl- or diphenyl-amino substituted thiophene stilbenes. Excellent tradeoffs among absorption, mol. nonlinearity and thermal stability were achieved. Electro-optic polymers based on the guest/host systems and covalent attachment of chromophores onto high temperature polyquinoline backbones demonstrated high E-O activities (T33 ≤ 28 pm/V at 1.3 µm) and good optical, elec. and mech. properties. 302965-26-DP 303031-08-5P RI: PRP (Properties), SPN (Synthetic preparation); PREP (Preparation) (design and synthesis of highly efficient chromophores and polymers

electro-optic applications)
302965-26-0 CAPLUS
Propanedintrile, 2-[[5-[2-[4-(dibutylamino)phenyl]ethenyl]-2-thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]- (CA INDEX NAME)

303031-08-5 CAPLUS
Propanedinitrile, [[5-[2-[4-[bis(butylphenyl]amino]phenyl]ethenyl]-2-thienyl](2,3,5,6-tetrafluoro-4-pyridinyl)methylene]- (9CI) (CA INDEX

L33 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
1997:332662 Document No. 127:25334 Original Reference No. 127:4819a,4822a
The role of London forces in defining noncentrosymmetric order of high
dipole moment-high hyperpolarizability chromophores in electrically poled
polymeric thin films. Dalton, Larry R.; Harper, Aaron W.; Robinson,

H. (Loker Hydrocarbon Res. Inst., Univ. Southern California, Los Angeles, CA, 90089-1661, USA). Proceedings of the National Academy of Sciences of the United States of America, 94(10), 4942-4947 (English) 1997. CODEN: PNRSA6. ISSN: 0027-8424. Publisher: National Academy of Sciences. Graphs of 2nd harmonic generation coeffs. and electrooptic coeffs. (measured by ellipsometry, attenuated total reflection, and 2-slit interference modulation) as a function of chromophore number d.

interference modulation) as a function of chromophore
loading) are exptl. observed to exhibit maxima for polymers containing
chromophores characterized by large dipole moments and polarizabilities.
Modified London theory is used to demonstrated that this behavior can be
attributed to the competition of chromophore-applied elec. field and
chromophore-chromophore electrostatic interactions. The comparison of
theor, and exptl. data explains why the promise of exceptional
macroscopic
2nd-order optical nonlinearity predicted for organic materials was not

pscopic
2nd-order optical nonlinearity predicted for organic materials was not realized and suggests routes for circumventing current limitations to large optical nonlinearity. The results also suggest extensions of measurements and theor, methods to achieve an improved understanding of intermol. interactions in condensed phase materials including materials prepared by sequential synthesis and block copolymer methods.
161419-15-4 161419-16-18

161419-15-4 161419-16-5
RL: MOA (Modifier or additive use), PRP (Properties); USES (Uses)
(London forces role in defining noncentrosym. order in elec. poled
polymeric films of high dipole moment-high hyperpolarizability)
161419-15-4 CAPLUS
Propanedinitrile, 2-[[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2thienyl]methylene]- (CA INDEX NAME)

161419-16-5 CAPLUS
Propanedinitrile, 2-[3-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]-2-propen-1-ylidene]- (CA INDEX NAME)

L33 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L33 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L33 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN 1995:820373 Document No. 123:353882 Original Reference No.

1995:820373 Document No. 123:333002 Original Netcount 123:63235a,63238a Large second-order optical nonlinearities and enhanced thermal stabilities
in extended thiophene-containing compounds. Gilmour, Sandra; Marder,

in extended thiophene-containing compounds. Gilmour, Sandra; Marder, Seth

R.; Perry, Joseph W.; Cheng, Lap Tak (Jet Propulsion Lab., California Inst. Technol., Pasadena, CA, 91109, USA). Advanced Materials (Weinheim, Germany), 6(6), 494-6 (English) 1994. CODEN: ADVMEW. ISSN: 0935-9648. Publisher: VCH.

AB In order to increase the degree of ground-state polarization, thiophene-containing compds. with a 3-phenyl-5-isoxarolone acceptor were prepared and their nonlinearities were compared to compds. with a dicyanovinyl acceptor. An enhanced nonlinearity and excellent long-term stability at 80° was observed

IT 161419-15-4

RL: PRP (Properties)
 (thiophene-containing compds. with large 2nd-order optical nonlinearities
 and enhanced thermal stabilities)

RN 161419-15-4 CAPIUS

CN Propanedinitrile, 2-[[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thienyl]methylene]- (CA INDEX NAME)

IT 161419-16-5P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (thiophene-containing compds. with large 2nd-order optical nonlinearities

and enhanced thermal stabilities)

and enhanced thermal stabilities, 161419-16-5 CAPLOS Propanedinitrile, 2-[3-[5-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]-2-propen-1-ylidene]- (CA INDEX NAME)

L33 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
1995;35025 Document No. 122:163483 Original Reference No. 122:30099a,30102a
Enhanced second-order optical nonlinearities in extended thiophene
containing compounds. Gilmour, Sandra; Marder, Seth R.; Perry, Joseph

Cheng, Lap-Tak (Jet Propulsion Laboratory, California Institute Technology, Pasadena, CA, 91109, USA). Proceedings of SPIE-The International Society for Optical Engineering, 2143(ORGANIC, METALLO-ORGANIC AND POLYMERIC MATERIALS FOR MONLINBAR OPTICAL APPLICATIONS), 117-23 (English) 1994. CODEN: PSISDG. ISSN: 0277-786X.

 $^\star$  structure diagram too large for display - available via offline print  $^\star$ 

AB The synthesis and first hyperpolarizabilities  $(\beta)$  of the donor-acceptor-substituted thiophene-containing compds. I, II, III, and ...

reported. III and IV, incorporating the acceptor group 3-phenyl-5-isoxazolone (that can gain aromaticity upon charge

3-phenyl-5-isoxazolone (that can gain aromaticity upon charge separation) had larger β than the analogous I and II mols. containing a dicyanovinyl acceptor. For both acceptors, insertion of a vinyl group between the thiophene bridge and methine carbon of the acceptor enhances the second-order hyperpolarizability but does not lead to a significant decrease in thermal stability. The mols. (1-2%) were incorporated into PMMA and the electro-optic coeffs. of these host-guest compns. measured. IT 161419-15-4P 161419-16-5P RL: PRP (Properties); SFN (Synthetic preparation); PREP (Preparation) (enhanced second-order optical nonlinearities in extended thiophene-containing compds.)

RN 161419-15-4 CAPLUS
CN Propanedinitrile, 2-[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thienyl]methylene]- (CA INDEX NAME)

L33 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Propanedinitrile, 2-[3-[5-[2-[5-(1-piperidiny1)-2-thieny1]etheny1]-2-thieny1]-2-propen-1-ylidene]- (CA INDEX NAME)

133 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2010 ACS on STN
1994:544723 Document No. 121:144723 Original Reference No.
121:25969a, 25972a
Second-order nonlinear optical properties of thiophene containing chromophores with extended conjugation. Gilmour, Sandray Jen, Alex K-Y.;
Marder, Seth R.; Neissink, A. Jennifer; Perry, Joseph W.; Skindhoej,
Joergen; Cai, Young Ming (Jet Propul. Lab., California Inst. Technol.,
Pasadena, CA, 91109, USA). Materials Research Society Symposium
Proceedings, 328(Electrical, Optical, and Magnetic Properties of Organic Solid State Materials), 485-90 (English) 1994. CODEN: MRSPDH. ISSN: 0272-9172.

AB The synthesis and first hyperpolarizabilities (β) of various donor-acceptor substituted thiophene containing compds with extended conjugation are reported. Results indicate that replacing Ph rings with less aromatic thiophene moieties enhances the second-order hyperpolarizability. Incorporating the acceptor group,
N,N'-diethylthiobarbituric acid, that can gain aromaticity upon charge-separation has also led to an increase in the nonlinearity. Some of the

charge-separation has also led to an increase in the nonlinearity. Some of the mols. have been incorporated into poly(Me methacrylate) and the electrooptic coeffs. of these host-guest polymers were measured.

IT 157300-03-3
RL: PRP (Properties)
 (second-order nonlinear optical properties of)
RN 157300-03-3 CAPLUS
CN Propanedinitrile, [[5-[2-[5-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]methylene]-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

=> s merocyanine

4027 MEROCYANINE

904 MEROCYANINES

L34 4286 MEROCYANINE

(MEROCYANINE OR MEROCYANINES)

 $\Rightarrow$  s 134 and review/dt

2385147 REVIEW/DT

L35 91 L34 AND REVIEW/DT

=> d scan ti

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
TI Phototherapeutic potential of alternative photosensitizers to porphyrins
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Organic colorants in light harvesting HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
TI Pharmacological purging of bone marrow with drugs other than
cyclophosphamide derivatives

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Dyes for dye diffusion thermal transfer (D2T2) printing

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Current topics in photochemistry of sensitizing dyes

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Merocyanine 540

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Recent progress in the study of ultra-thin films

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L35 91 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
TI Dye-based organogels: Stimuli-responsive soft materials based on one-dimensional self-assembling aromatic dyes

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

L11

L12

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=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
    FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
               STRUCTURE UPLOADED
L1
             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
L10
             0 S L3 AND L9
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26 S ELECTRO-OPTIC CHROMOPHORES

12 S L4 OR L9

L29 L30	FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35	FILE 'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT
=> s L36	135 and furna 2 FURNA 119 FURNAS 120 FURNA (FURNA OR FURNAS) 0 L35 AND FURNA
=> s	135 and furan 49439 FURAN 8356 FURANS 53345 FURAN (FURAN OR FURANS)
L37	0 L35 AND FURAN

- L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
  TI Flash photolysis study of the mechanism of photocoloring of spiropyrans of

the naphtho[1,8-b,c]furan series

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
  TI Furan substituted thiazoles and selenazoles and sensitizing dyes
  therefrom

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN

TI Chemistry of 1,8-substituted naphthalenes. III. Synthesis of salts of 2-(4'-methoxy-8'-hydroxy-1'-naphthyl)benzopyrylium and photochromic 5-methoxynaphtho[1,8-b,c]furan-2-spiro-2'-[2H]chromenes from them

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI A Tubular Biocontainer: Metal Ion-Induced 1D Assembly of a Molecularly Engineered Chaperonin

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Merocyanine dyes

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

138 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN

TI Structure-property dependence of the first hyperpolarizabilities of organometallic merocyanines based on the μ-vinylcarbynediiron acceptor and ferrocene doπor

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
TI Chemical and chemotherapeutic studies on furan derivatives.
XXIV. 3-Amino-as-triazine derivatives

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Effect of heteroaromatic annulation with five-membered rings on the photochromism of 2H-[1]-benzopyrans

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L38 9 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN TI Solvent effects in merocyanine spectra

ALL ANSWERS HAVE BEEN SCANNED

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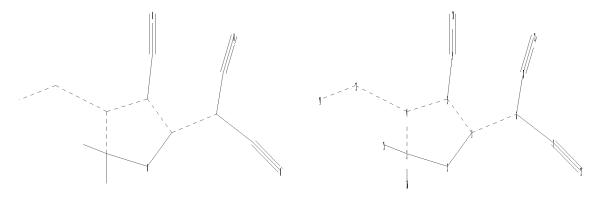
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http://www.cas.org/support/stngen/stndoc/properties.html

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chain nodes : 6 7 8 9 ring nodes : 1 2 3 4 5 ring/chain nodes : 10 11 12 13 14 15 16 chain bonds :  $1-6 \quad 3-15 \quad 3-16 \quad 4-13 \quad 5-9 \quad 6-7 \quad 6-8 \quad 7-12 \quad 8-11 \quad 9-10$ ring/chain bonds : 13 - 14ring bonds : 1-2 1-5 2-3 3-4 4-5 exact/norm bonds :  $1-2 \quad 1-5 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-13 \quad 7-12 \quad 8-11 \quad 9-10 \quad 13-14$ exact bonds : 3-15 3-16 5-9 6-7 6-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS

50 ANSWERS

## L39 STRUCTURE UPLOADED

=> s 139

SAMPLE SEARCH INITIATED 16:06:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 57 TO ITERATE

100.0% PROCESSED 57 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 688 TO 1592
PROJECTED ANSWERS: 608 TO 1472

L40 50 SEA SSS SAM L39

=> d scan

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C42 H54 N4 O3 S2 S12

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20000

PAGE 2-B

PAGE 2-A

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 4-[[4-[1,1-bis[4-[[4[(trifluoroethenyl)oxy]phenyl]methoxy]phenyl]ethyl]phenoxy]methyl]-,
[[4-[2-[3-[3-[4-cyano-5-(dicyanomethylene)-2-[4-[[(1,1dimethylethyl)dimethylsilyl]oxy]butyl]-2,5-dihydro-2-methyl-3-furanyl]-2-

PAGE 1-A

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1,2-Benzenedicarboxylic acid,
1-[6-[4-4-[5-[2-2-[3-[3,5-biz[[4-[(1,2,2-trifluoroethenyl) oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester

MF C69 H58 F6 N4 Oll S
C1 CCM

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
[3-cyano-4-[(1E)-2-[3,4-diethyl-5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF C33 H36 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Acetamide, N-[6-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3furanyl]-1,3,5-hexatrien-1-yl]-N-phenyl
MF C24 H20 N4 O2

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[4-[2-[5-[2-[4-[bis (4-iodophenyl)amino]phenyl]=thenyl]2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C36 H24 I2 N4 O S
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[2-[5-[2-[1-(phenylmethyl)-1H-indol-3-yl]ethenyl]-2-thienyl]ethenyl]-2(5H)-furanylidene]-MF C33 H24 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[[6-[(1,1-dimethylethyl-dimethylethyl-dimethylethyl-dimethylethyl-dimethylethyl-dimethylethyl-dimethylethyl-dimethyl-dimethyl-dimethyl-dimethyl-dimethyl-dimethyl-dimethyl-dimethyl-5-(trifluoromethyl)-2-thlenyl-furanyl-dimethyl-2-thlenyl-5-methyl-5-(trifluoromethyl)-2(5H)-furanyl-dimethyl-di

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[6-(dihexylamino)-2-naphthalenyl]-5-(3-hydroxypropyl)-5-methyl-2(5H)-furanylidene]
MF C34 H42 N4 O2

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Acetamide,
N=[[2-chloro-3-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-5-(1,1-dimethylethyl)-2-cyclohexen-1-ylidene]methyl]-N-phenylMF C31 H31 C1 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1Z,3E)-3-[3-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-methoxy-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C32 H34 N4 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

TN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[1-(phenylmethyl)-1H-pyrrol-2-yl]ethenyl]-2(5H)-furanylidene]
MF C23 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[(1-oxo-2-propen-1-yl)oxy]-,
[5-[2-[4-[[2-[[3,5-bis[(1-oxo-2-propen-1-yl)oxy]-yl)oxy]benzoyl]oxy]ethyl]ethylamino]phenyl]ethenyl]-2-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-3-thienyl]methyl ester

MF C55 H41 F3 N4 013 S

PAGE 2-A

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-(dimethylamino)ethenyl]-5,5-dimethyl2(5H)-furanylidene]NF C14 H14 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[2-chloro-3-[2-(1-decyl-4(1H)-

Double bond geometry as described by E or Z.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzoic acid, 3,5-bis(phenylmethoxy)-,

[[4-[2-[4-[[[3,5-bis(phenylmethoxy)benzoyl]oxy]methyl]-5-[2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI)
MF C38 H88 N4 O13 S

PAGE 1-B

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-(4-chlorophenyl)ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]MF C18 #12 C1 N3 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, [3-cyano-4-[(12)-2-[[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-7-[(12)-2-[4-[ethyl(2-hydroxyethyl)aminolphenyl]ethenyl]-2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yllethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (9CI)

MF C37 H44 N4 O5 S Si

CI IDS

PAGE 2-A о— сн<sub>2</sub>— р1 si-Bu-t

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S Si

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 O5 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(3,4-dimethylphenyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C48 H50 N4 O 8

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Acetanide, N-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-N-phenylNF C20 H16 N4 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1H-Pyrrole-1-propanoic acid, 2,5-dihydro-2,5-dioxo-,

2-[[4-[2-[3-[[[3,5-bis[(2,3,4,5,6-pentafluorophenyl)methoxy]benzoyl]oxy]methyl]-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylamino]ethyl ester

MF C57 H36 F13 N5 O9 S

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CM 5

•2 HCl

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1N 1,3-Isobenzofurandione, 5,5'-[2,2,2-trifluoro-1(trifluoromethyl)ethylidene]bis-, polymer with 2,4-diaminophenol
dihydrochloride, 6-[(4-[(12)-2-[3,4-dibutoxy-5-[(18)-2-[3,4-dibutoxy-5[(18)-2-[4-cymno-5-didyanomethylene)-2,5-dihydro-2-methyl-2-[3-[(4[(trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylamino]hexyl

(ester)

(ester)

MF C73 H81 F3 N4 O12 S2 . x (C19 H6 F6 O6 . C6 H8 N2 O . 2 C1 H)x . x C9 H5
F3 O3

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[4-[5-[butyl[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-

y1)ethy1]amino]-2-thieny1]pheny1]-3-cyano-5,5-dimethy1-2(5H)-furanylidene]-MF C30 H27 N5 O3 S

PAGE 1-A

PAGE 2-A

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-4-(1-hexyl-1,2,3,4-tetrahydro-6-quinolinyl)5,5-dimethyl-2(5H)-furanylidene]
MF C25 H28 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[2-chloro-5-(1,1-dimethylethyl)-3-[2-(1-hexyl-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene)ethylidene]-1-cyclohexen-1-yllethenyl|-3-cyann-5,5-dimethyl-2(5H)-furanylidene]
MF C40 H47 C1 N4 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Propanedinitrile,
2-[3-cyano-4-[(1E,7E,5E,7E)-8-[4-(dimethylamino)phenyl]1,3,5,7-octatetraen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]MF C26 H24 N4 0

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-3-[3-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-2-methoxy-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C32 H34 N4 O2

Double bond geometry as shown.

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Acetamide, N-[5-[bis(2-hydroxyethyl)amino]-2-[2-[3,4-dibutoxy-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]diazenyl]phenyl]
MF C36 H43 N7 06 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[2-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-5-thiazolyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidenelMF C25 H21 N5 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[4-[ethyl(2-hydroxyethyl)amino]phenyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C22 H22 N4 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[5,5-dibutyl-3-cyano-4-[3-[3-[2-[4-

(dibutylamino)phenyl]ethenyl]-2-hexyl-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-2(5H)-furanylidene]-MF C49 H68 N4 O

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-(3,4-dihydroxyphenyl)ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C18 H13 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[3-[3-[2-[4-[bis(2-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[(1E,3E)-3-[3-[(1E)-

2-[4-(diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-5-methyl-2(5H)-furanylidene]MF C44 H48 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[4-[hexadecyl[12-(4-hexadecyl-2,5-dioophenyl]) dodecyl]amino]phenyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C68 H104 12 N4 O

C70 C0M

Double bond geometry as shown.

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C34 H33 F3 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,4,5-tris[(2-ethylhexyl)oxy]-,
[8-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-8-'-[[12-2-4-(dibutylamino)phenyl]ethenyl][6,6'-bi-2H-thieno[3,4-b][1,4]dioxepin]-3,3'(4H,4'H)-diylidene]tetrakis(methylene)
ester (9CI)

MF C170 H260 N4 025 S2

Double bond geometry as shown.

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-3-[3-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C33 H36 N4 O

Double bond geometry as shown.

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[4-[[2-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E,3E)-3-[(1E)-2-[4-[bis(4-

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[butyl[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)furanylidene]MF C26 H25 N5 03 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[2-chloro-3-[2-[1,3-dihydro-3,3-dimethyl-1-(phenylmethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-dimethylethyl)-1-cyclohexen-1-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H41 C1 N4 O

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[(1E,3E,5E,72)-8-cyano-8-[4-(dimethylamino)phenyl]-1,3,5,7-octatetraen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]MF C27 H23 N5 0

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2=[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-(4-butylphenyl)ethenyl]]-2-thiazolyl]ethenyl]-2-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C33 H28 N4 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COFFRIGHT 2010 ACS on STN

Benzenebutanoic acid, 4-hydroxy-y-(4-hydroxyphenyl)-y-methyl-,
polymer with 1,1'-sulfonylbis[4-chlorobenzene],
2-[[4-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3furanyl]ethenyl]phenyl]ethylamino]ethyl ester

MF C22 H22 N4 O2 . x (C17 H18 O4 . C12 H8 C12 O2 S)x

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 2 CM 3

CM 4

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued) \*\*PROPERTY DATA AVAILABLE IN THE "PROP" FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[3-[3-[2-(4-aminophenyl)ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C29 H28 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L40 50 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-(2-hydroxyphenyl)ethenyl]-5,5dimethyl-2(5H)-furanylidene]
MF C18 H13 N3 02

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

L10

L11

L12

```
=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
    FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
               STRUCTURE UPLOADED
L1
             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
```

26 S ELECTRO-OPTIC CHROMOPHORES

0 S L3 AND L9

12 S L4 OR L9

```
FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010
         90 S L27
L29
L30
            13 S L28
    FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010
L31
            1 S L27 AND HYDROXYETHYL
    FILE 'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010
            6 S L31
            19 S L32 OR L30
L33
L34
          4286 S MEROCYANINE
L35
            91 S L34 AND REVIEW/DT
L36
             0 S L35 AND FURNA
L37
             0 S L35 AND FURAN
L38
             9 S L34 AND FURAN
    FILE 'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
    FILE 'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010
L39 STRUCTURE UPLOADED
L40
            50 S L39
=> s 139 full
FULL SEARCH INITIATED 16:07:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1024 TO ITERATE
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L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[2-[(1E)-2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-5-thiazolyl]ethenyl]-2(5H)-furanylidene]
MF C26 H23 N5 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):111

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[2,2':6',2''-terpyridin]-4'-ylethenyl]-2(5H)-furanylidene]
MF C27 Hi8 N6 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1-Butanaminium, N,N,N-tributyl-, salt with 2-[4-[2-[3-[2-[4-cyano-5-(dicyanomethyl)-2,2-dimethyl-3(2H)-

CM 2

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenesulfonic acid, 4-methyl-, compd. with
2-(3-cyano-5,5-dimethyl-4-(2-[1-methyl-5-(1-piperidinyl)-1H-pyrrol-2y1]ethenyl]-2(5H)-furanylidene]propanedinitrile, ion(1-) (1:1)

MF C22 H23 N5 O . C7 H7 O3 S

CM

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS ON STN IN INDEX NAME NOT YET ASSIGNED

MF C28 H28 N4 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[7-(1-methyl-2(1H)pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]
MF C23 H20 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[3-[1-(2-hydroxyethyl)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
NF C20 H18 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[7-(1-methyl-4(1H)pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]
MF C23 H20 N4 O

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E,8E)-8-(1-methyl-2(1H)-pyridinylidene)-2,4,6-octatrien-1-yl]-2(5H)-furanylidene]MF C24 H22 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[2-(3-pyridinyl)ethenyl]-2(5H)-furanylidene)
MF C17 H12 N4 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2=[3-cyano-5,5-dimethyl-4-[(1E,3E)-5-(1-methyl-4(1H)pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene]
MF C21 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-eyan-5,5-dimethy]-4-[(1E)-2-[2-[(1E)-2-[1-methy]-5(1-piperidiny])-1H-pyrrol-2-yl]ethenyl]-5-thiazolyl]ethenyl]-2(5H)furanylidene]
MF C27 H26 N6 O S

Double bond geometry as shown.

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-(1-piperidinyl)ethenyl]-2(5H)-£uranylidene]CT TH8 N4 O
CT CCM

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-[1-methyl-5-(1-piperidinyl)-1H-pyrrol-2-yl]ethenyl]-2(5H)-furanylidene]-NF C22 H23 N5 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-3-[2-[4-cyano-5-(dicyanomethyl)-2,2-dimethyl-3(2H)-furanylidene]ethyl]-5-(1,1-dimethylethyl)-2-(1-piperidinyl)-1-cyclohexen-1-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-, ion(1-)

WF C39 H42 N7 O2

CI CCM

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED

MF C32 H36 N4 O2

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

| P-Alanine, N-[4-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dinethyl-3-furanyl]ethenyl]-| N-methyl-1,
| 2-[4,5-dihydro-4-[(1-methyl-4(1H)-pyridinylidene)ethylidene]-5-oxo-3-propyl-1H-pyrazol-1-yl]ethyl ester (9CI)

MF C38 H39 N7 04

PAGE 1-B

\_ Dr\_1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[5-(1-methyl-4(1H)pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene]
MF C21 H18 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[5-(1-methyl-2(1H)-pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene]
NF C21 H18 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E)-6-(1-methyl-2(1H)pyridinylidene)-2,4-hexadien-1-yl]-2(5H)-furanylidene]MF C22 H20 N4 O

Double bond geometry as shown.

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[(1E)-3-[1-[2-(acetyloxy)ethyl]-4(1H)-pyridinylidene]-1-propen-1-yl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C22 H20 N4 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-(3-cyano-5,5-dimethyl-4-[2-(2-pyridinyl)ethenyl]-2(5H)furanylidene)
MF C17 H12 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[2-chloro-3-[2-(1-decyl-4(1H)-

Double bond geometry as described by E or Z.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2=[3-cyano-5,5-dimethyl-4-[(1E)-2-(1-piperidinyl)+cfs)-furanylidene]-, hydrate (50:19)
MF C17 H18 N4 0 . 19/50 H2 0

Double bond geometry as shown.

●19/50 H<sub>2</sub>O

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[7-(1-ethyl-4(1H)-pyridinylidene)-1,3,5-heptatrien-1-yl]-5,5-dimethyl-2(5H)-furanylidene)MF C24 H22 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED

MF C24 H20 N4 0

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzenesulfonic acid, 4-methyl-, compd. with
2-[3-cyano-5,5-dimethyl-4-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2(5H)furanylidene]propanedintrile, ion(1-) (1:1)

MF C21 H20 N4 O S . C7 H7 O3 S

CM 1

CM S

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[4-(3,5-dimethyl-1-piperidinyl)phenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C23 H24 N4 O

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[3-(1-methyl-2(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]MF C19 H16 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

NC-C CN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]
NF C19 H16 N4 0

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E)-4-(1-methyl-2(1H)-pyridinylidene)-2-buten-1-yl]-2(5H)-furanylidene]
MF C20 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-3-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C21 H20 N4 O3

Double bond geometry as shown.

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[4-[(1E)-2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2-thiazolyl]ethenyl]-2(5H)-furanylidene]
MF C26 H23 N5 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile,  $2-3-\mathrm{copanedinitrile},\\ 2-3-\mathrm{copaned-1-3-(1-decyl-4(1H)-pyridinylidene)-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-}$  MF C28 H34 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-4-(1-piperidinyl)-1,3-butadien-1-yl]-2(5H)-furanylidene]-MF C19 H20 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED

MF C35 H40 N4 O3

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-{3-cyano-5,5-dimethyl-4-{2-{5-(1-piperidinyl)-2-thienyl}j-2(5H)-furanylidene}
MF C21 H20 N4 O S
CC CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[7-[1-(2-hydroxyethyl)-4(1H)-pyridinylidene]-1,3,5-heptatrien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C24 H22 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[5-[1-(2,3-dihydroxypropyl)-2(1H)pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C23 H22 N4 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-4-[5-[1-(2,3-dihydroxypropyl)-4(1H)pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C23 H22 N4 O3

L42 54 ANSWERS REGISTRY COPPRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[(2E,4E,6E)-6-[1-(2,3-dihydroxypropyl)-

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]
MF C19 H16 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-5-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C23 H22 N4 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[5-[(1E)-2-[1-methyl-5(1-piperidinyl)-1H-pyrrol-2-yl]ethenyl]-2-thienyl]ethenyl]-2(5H)MF C28 H27 N5 O S

Double bond geometry as shown.

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-(3-cyano-4-[(1E)-2-(3,5-di-2-pyridinylphenyl)ethenyl]-5,5-dimethyl-2(5H)-furanylidene)MF C28 H19 N5 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED

MF C32 H36 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Butanedioto acid, 1,1'-[1-[(4-[2-(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4H-pyracol-4-ylidene)ethylidene]-1(4B)-pyridinyl)methyl]-1,2-ethanediyl]
4,4'-bis[2-[(4-[(1E)-2-(4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]phenyl]methylamino]ethyl] ester

MF C70 H65 N11 O11

Double bond geometry as described by E or  $\ensuremath{\mathtt{Z}}\xspace$  .

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED
MF C28 H15 F13 N4 O

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[5-[1-(2-hydroxyethy1)-4(1H)-pyridinylidene]-1,3-pentadien-1-y1]-5,5-dimethy1-2(5H)-furanylidene]MF C22 H20 N4 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[3-[1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]NF C21 H20 N4 03

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-4-[3-[1-(2,3-dihydroxypropyl)-4(1H)pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C21 H20 N4 03

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(2E,4E)-4-[1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene]-2-buten-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C22 H22 N4 03

Double bond geometry as shown.

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E,3E,5E)-7-(1-methyl-4(1H)pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]MF C23 H20 N4 0

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L42 54 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-eyano-5,5-dimethyl-4-[2-(4-pyridinyl)ethenyl]-2(5H)-furanylidenel |
MF C17 H12 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

L28

=> d his (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010) FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 L1 STRUCTURE UPLOADED L2 0 S L1 L3 14 S L1 FULL FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 L411 S L3 FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010 FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5TRA L4 1- RN : 172 TERMS FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 172 SEA L5 L6 L7 1 S L3 NOT L6 FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 L8 0 S OTOPHORE L9 1 S OPTOPHORE L10 0 S L3 AND L9 L11 12 S L4 OR L9 L12 26 S ELECTRO-OPTIC CHROMOPHORES L13 0 S ELECTROPTIC CHROMOPHORES L1427 S ELECTROOPTIC CHROMOPHORES L15 11072 S ELECTROOPTIC L16 660 S L15 AND CHROMOPHORE 679 S L12 OR L14 OR L16 L17 FILE 'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010 L18 269403 S C6N/RF FILE 'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010 TRA L17 1- RN : L19 3023 TERMS FILE 'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 L20 214 S L20 AND C5N/RF L21 L22 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE L23 25 S L22 OR L23 L24 L25 25 S L24 NOT L3 FILE 'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25 L26 FILE 'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010 FILE 'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 L27 6 S L25 AND 5<=REF.CAPLUS

19 S L25 NOT L27

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L29
             90 S L27
L30
             13 S L28
     FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010
L31
              1 S L27 AND HYDROXYETHYL
     FILE 'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010
L32
              6 S L31
L33
             19 S L32 OR L30
           4286 S MEROCYANINE
L34
L35
             91 S L34 AND REVIEW/DT
L36
              0 S L35 AND FURNA
L37
              0 S L35 AND FURAN
L38
              9 S L34 AND FURAN
     FILE 'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
     FILE 'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010
L39
               STRUCTURE UPLOADED
L40
             50 S L39
L41
            947 S L39 FULL
L42
             54 S L41 AND C5N/RF
=> file caplus
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FILE 'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010

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FILE COVERS 1907 - 7 Jun 2010 VOL 152 ISS 24

FILE LAST UPDATED: 6 Jun 2010 (20100606/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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=> s 142 L43 20 L42

=> d cbib abs hitstr 1-YOU HAVE REQUESTED DATA FROM 20 ANSWERS - CONTINUE? Y/(N):y

L43 ANSWER 1 OF 20 CAPLUS COPPRIGHT 2010 ACS on STN 2010:304297 Document No. 152:556918 Toward highly efficient NLO chromophores: Synthesis and properties of heterocycle-based

chromophores: Synthesis and properties of heterocycle-based electronically gradient dipolar NLO chromophores: Ma, Xiaohua; Ma, Fei; Zhao, Zhenhua; Song, Naiheng; Zhang, Jianping (Beijing National Laboratory for Molecular Sciences, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Department of Polymer Science and Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, Peop. Rep. China). Journal of Materials Chemistry, 20(12), 2369-2380 (English) 2010. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB To realize organic nonlinear optical (NLO) chromophores with optimized ground-state polarization and very large mol. optical nonlinearities, a novel series of heterocycle-based electronically gradient dipolar chromophores were designed and synthesized. These chromophores are featured by their same strong electron acceptor (i.e., 2-dioyanomethylene-3-cyano-4, 5,5-trimethyl-2,5-dihydrofuran, TCF) and the same length of x-conjugation, but different electron donors (e.g., dialkylamine and dianisylamine), different (heterolarons. with varying electron densities (i.e., pyrrole, thiophene, and benzene) as the auxiliary donor, and electron-poor 1, 3-heteroarom. thiazole with different

auxiliary donor, and electron product of deferent regiostructures (e.g., either electron-poor C2, "matched", or electron-rich C5, "un-matched", is connected to the acceptor) as the auxiliary acceptor, which allows for a systematic fine-tuning of the ground-state polarization. The gradient electronic structures and optical

ral properties of these NLO chromophores were carefully characterized by 1H NME, CV, UV-vis, and Hyper-Rayleigh scattering expts. All the NLO chromophores exhibited very large static mol. first hyperpolarizabilities ( $\beta$ 0) in the range of 450-950 + 10-30 esu, which showed significant dependence on the gradient electronic structures. Upon using electron-rich heteroarom. cycle as the auxiliary donor, "matched"

thiazole

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN

(Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PRCC (Process); USES (Uses) (toward highly efficient NLO chromophores and synthesis and properties of heterocycle-based electronically gradient dipolar NLO chromophores) 1225601-90-0 CAPLUS Propanedinitrile, -cyano-5,5-dimethyl-4-[(1E)-2-[2-[(1E)-2-[1-methyl-5-(1-piperidinyl)-1H-pyrrol-2-yl]ethenyl]-5-thiazolyl]ethenyl]-2(5H)-

L43 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[4-[(1E)-2-[5-(1-

piperidiny1)-2-thieny1]etheny1]-2-thiazoly1]etheny1]-2(5H)-furanylidene](CA INDEX NAME)

Double bond geometry as shown.

L43 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN furanylidene] - (CA INDEX NAME) (Continued)

Double bond geometry as shown.

1225601-91-1 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[2-[(1E)-2-[5-(1-

piperidiny1) -2-thieny1]etheny1]-5-thiazoly1]etheny1]-2(5H)-furanylidene](CA INDEX NAME)

Double bond geometry as shown.

1225601-92-2 CAPLUS
Propanedinitrile,
-cyano-5,5-dimethyl-4-[(1E)-2-[5-[(1E)-2-[1-methyl-5(1-piperidinyl)-1H-pyxrol-2-yl]ethenyl]-2-thienyl]ethenyl]-2(5H)furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

1225601-98-8 CAPLUS

L43 ANSMER 2 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2009:728784 Document No. 151:256964 The effects of oxygen concentration and
light intensity on the photostability of zwitterionic chromophores.
Raymond, S. G.; Williams, G. V. M.; Lochocki, B.; Bhuiyan, M. D. H.; Kay,
A. J.; Quilty, J. W. (Photonics Group, Industrial Research Ltd., Lower
Hutt, 5040, N. 2.) Journal of Applied Physics, 105(11),
113123/1-113123/7 (English) 2009. COMEN: JAPIAU. ISSN: 0021-8979.
Publisher: American Institute of Physics.
AB Photostability measurements at different oxygen partial pressures and
light intensities have been made on host-quest films containing amorphous
polycarbonate and an organic chromophore with a high second order
nonlinear

due to a reduced oxygen content in the film caused by chromophore photodegrdn. rather than ground state bleaching. There is an anomalous increase and then decrease in the photoluminescence intensity that cannot easily be explained. (c) 2009 American Institute of Physics.

IT RL: PEP (Physical, engineering or chemical process); PRP (Properties);

RCT
(Reactant); PROC (Process); RACT (Reactant or reagent)
(effects of oxygen concentration and light intensity on
photostability of
zwitterionic chromophores in host-guest films containing amorphous

zwitterionic chromophores in nost-guest films contains polycarbonate)

RN 1178886-26-4 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[3-(14-decyl-4(1H)-pyridinylidene)-1-propen-1-y1]-5,5-dimethyl-2(5H)-furanylidene)- (CA INDEX NAME)

ANSWER 3 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 9:667202 Document No. 151:2212840 Preparation and characterization of second order non-linear optical properties of new "push-pull" platinum complexes. Scarpaci, Annabelle; Monnereau, Cyrille; Herque, Noemie; Blart, Errol; Legoupy, Stephanie; Odobel, Fabrice; Gorfo, Ayele; Perez-Moreno, Javier; Clays, Koen; Asselberghs, Inge (CEISAM, Chimie Et Interdisciplinarite, Synthese, Analyse, Modelisation, UFR des Sciences et des Techniques, Universite de Nantes, May22, Fr.). Dalton Transactions (23), 4538-4546 (English) 2009. CODEN: DTARAF. ISSN: 1477-9226. OTHER SOURCES: CASREACT 151:221284. Publisher: Royal Society of Chemistry. 2009:667202 of Chemistry.

Platinum pincer terpyridine and di-2-pyridylphenyl chloro and acetylide complexes substituted by 2-cyanobutenolide and  $\alpha_1\alpha_2$ -pyingspheny under an accyline complexes substituted by 2-cyanobutenolide and  $\alpha_1\alpha_2$ -tricyano-2-methylenedihydrofuran chromophores were prepared and characterized by UV and non-linear optical data. The new platinum complexes I or I-PF6 [9-12; X = cl, 15, X = C.tplbond.c-1,4-C6H4N(C6H13)2; 18, C.tplbond.c-1,4-C6H4N(C6H13)2; 18,

= C.tplkond.CPh; 9, 11, 15, 16, 18, Z = 0, 10, 12, Z = :C(CN)2; Y = N, n

1; Y = C, n = 0] consist of a tridentate terpyridine or dipyridylphenyl ligand substituted by a strong electron accepting butenolide unit, and a chloro or an arylacetylide ligand. The hyper-Rayleigh scattering measurements reveal that these complexes display large quadratic hyperpolarizabilities reaching a dynamic value of 1460 + 10-30 at 1064 mm esu for the best complex. This investigation also demonstrates that cyclometalated dipyridylphenyl platinum complexes greatly exhibit enhanced first hyperpolarizability with respect to analogous terpyridyl complexes.

complexes.

IT 1174582-05-8P 1174582-06-9P
RL: KCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and nonlinear optical properties of platinum pincer terpyridine

and di-2-pyridylphenyl push-pull complexes substituted by

L43 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2009;207480 Document No. 150:2595450 Molecular Design and Synthesis of
Hetero-trichromophore for Enhanced Monlinear Optical Activity. Gao,
Junkuo; Cui, Yuanjing; Yu, Jiancan; Wang, Zhiyu; Wang, Minquan; Qiu,
Jianrong; Qian, Guodong (Department of Materials Science and Engleering,
State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou,
310027, Peop. Rep. China). Macromolecules (Washington, DC, United
States), 42(6), 2198-2203 (English) 2009. CODEM: MAMOSX. ISSN:
0024-9297. OTHER SOURCES: CASREACT 150:259545. Publisher: American
Chemical Society.

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

A new hetero-trichromophore (HT-1) (I) was designed and synthesized by linking neutral-ground-state (NGS) chromophore 1 (II) with zwitterionic (ZWI) chromophore 2 (III), and their mol. structures were confirmed yelemental anal., UV-vis absorption spectra, 1H NMR, etc. Theor. calons. show that there is a decrease of mol. dipole moments in gas phase when chromophores 1 and 2 are linked together. The polymer films were fabricated by doping trichromophore HT-1, NOS chromophore 1, and ZWI chromophore 2 into poly (4-vinylphenol) (FVPh). The second harmonic generation coeffs. (d33) of the films and the thermal stability of optical

onlinearities were measured by in situ second harmonic generation (SHG)
measurement. The results show that almost a 5-fold enhancement in second
harmonic coeffs. (d33) is realized as the combination of NGS chromophore
and ZWI chromophore. The results indicate that NGS and ZWI chromophore
combined hetero-trichromophores can efficiently improve the macroscopic
optical nonlinearities in poled polymer materials.
1070879-12-7P
RL: MCA (Modifier or additive use), PRP (Properties); SPN (Synthetic
preparation), PREP (Preparation); USES (Uses)
(zwitterion, poly(vinylphenol) doped with, mol. design and synthesis

TT

of hetero-trichromophore for enhanced nonlinear optical activity)

Double bond geometry as described by E or Z.

L43 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continuous Continuous Co (Continued)

11/482-U5-8 CAPLUS Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[2,2':6',2''-terpyridin]-4'-ylethenyl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 1174582-06-9 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[(1E)-2-(3,5-di-2-pyridinylphenyl)ethenyl]5,5-dimethyl-2(5H)-furanylidene)- (CA INDEX NAME)

Double bond geometry as shown.

L43 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-A

ANSWER 5 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
3:93768 Document No. 152:487904 Strategies for optimizing the
second-order nonlinear optical response in zwitterionic merocyanine dyes.
Teshome, Ayele; Kay, Andrew J.; Woolhouse, Anthony D.; Clays, Koen;
Asselberghs, Inge; Smith, Gerald J. (Department of Chemistry, University
of Leuven, Louvain, B-3001, Belg.). Optical Materials (Amsterdam,
Netherlands), 31(4), 575-582 (English) 2009. CODEN: CMATET. ISSN:
0925-3461. Publisher: Elsevier B.V..
The mol. linear and nonlinear optical (NLO) properties of a series of
seven merocyanine dyes have been studied in solvents covering a broad
range of polarity (dioxane to dimethylsulfoxide). The benchmark for the
series was the "Right hand side" zwitterionic chromophore 1, with a short
conjugation path and 4-pyridinylidene as the donor group. Optimization
strategies to improve the nonlinear response involved an extension of the
conjugation path (with one or two ethenyl groups), annelation (pyridine

quinoline), variation of the solvent polarity and partial ring locking of the x-conjugated system. All chromophores have as the acceptor moiety the cyanodicyanomethylidenedihydrofuran heterocycle. Optimizing the NLO response of these zwitterionic dyes by decreasing the polarity of the solvent is only possible for the parent chromophore 1. This is because the three other successful strategies employed to further improve the second-order NLO response in polar media, result in detrimental aggregation in nonpolar media. 1178886-26-4P 1222190-29-5P RL: PEP (Physical, engineering or chemical process); PRP (Properties);

SPN

(Synthetic preparation); PREP (Preparation); PRCC (Process)
(strategies for optimizing second-order nonlinear optical response in zwitterionic merocyanine dyes)

RN 117888-26-4 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[3-(1-decyl-4(1H)-pyridinylidene)-1-propen-1-y1]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

1222190-29-5 CAPLUS

Propanedinitrile, 2-[4-[(1E)-2-[2-chloro-3-[2-(1-decyl-4(1H)-

pyridinylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

L43 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 2008:1169221 Document No. 149:4714710 Process for preparation of second-order nonlinear optical chromophore compound. Qian, Guodong; Gao, Junkuo; Cui, Yuanjing; Chen, Lujian; Jin, Xuefeng; Wang, Zhiyu; Fan, Xianping; Wang, Minquan (Zhejiang University, Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 101270116 A 20080924, 9pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 2010-61316 20080422.

This invention provides a process for the preparation of I, composed of

neutral chromophores and one amphoteric ionic chromophore via covalent neutral chromophores and one amphoteric ionic chromophore via covalent bonds, as second-order nonlinear optical material. For example, 4-[(2-hydroxyethyl) (methyl)amino]benzaldehyde was reacted with 3-cyano-2-dicyanomethylene-4,5,5-trimethyl-2,5-dihydrofuran, followed by addition of succinic anhydride and 4-[(1-(2,3-dihydroxypropyl)-4(IH)-pyridinylidene]ethylidene]-2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one (preparation given) to give I in moderate yield. I has high rpolarization

hyperpolarization given; to give I in moderate yield. I has in hyperpolarization rate, small dipole moment, and high pyrolysis temperature IT 1070879-12-7P

1070879-12-7P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PEP (Preparation); USES (Uses)
(preparation of second-order nonlinear optical compound)
1070879-12-7 CAPLUS
Butanedioic acid, 1,1'-[1-[[4-[2-(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4H-pyraol-4-y-liden)e-tehylidene]-1(4H)-pyridinyl]methyl-1,2-ethanediyl]
4,4'-bis[2-[[4-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]phenyl]phenyl]methylamino]ethyl) ester (CA INDEX NAME)

Double bond geometry as described by E or Z.

L43 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L43 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-A

L43 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2008:1096944 Document No. 149:4498010 Stable near-infrared anionic
polymethine dyes: Structure, photophysical, and redox properties. Bouit,
Pierre-Antoine; Di Piazza, Emmanuel; Rigaut, Stephane; Le Guennic, Boris;
Aronica, Christophe; Touper, Loic; Andraud, Chantal; Maury, Olivier
(Laboratoire de Chimie, UNR 5182 CNRS, University of Lyon, Ecole Normale
Superieure de Lyon, 1900, 7, Fr.). Organic Letters, 10(19),
4159-4162 (English) 2008. CODEN: ORLEF7. ISSN: 1523-7060. OTHER SOURCES: CASREACT

149:449801. Publisher: American Chemical Society.

AB The concept of cyanine has been successfully extended to an anionic heptamethine dye featuring tricyanofuran moleties in terms of structure, reactivity, and photophys, properties. Importantly, absorption and emission are red-shifted compared to its classical cationic analog without any cost in terms of thermal stability. In addition to its "cyanine" behavior, this mol. exhibits further redox properties: oxidation and reduction CASREACT any cost in color of the behavior, this mol. exhibits further redox properties: oxidation and reduction
led to the reversible formation of radical species whose absorption is in marked contrast with that of cyanines.

IT 1068018-35-8P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(blue dye; preparation and properties of stable near-IR anionic polymethine
dyes)
RN 1068018-35-8 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, salt with
2-[4-[2-[3-[2-[4-cyano-5-(dicyanomethyl)-2,2-dimethyl-3(2H)furanylidene]ethyl]-5-(1,1-dimethylethyl)-2-(1-piperidinyl)-1-cyclohexen-1-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]propanedinitrile (1:1) (CA INDEX NAME) CM 1 CRN 1068018-34-7 CMF C39 H42 N7 O2

L43 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2008:1010609 Document No. 149:2785450 Organic nonlinear optical material of
nitrogen-containing heterocyclic compound, formation of nonlinear optical
polymer film, and optical modulator. Kawamonzen, Yoshihiro (Tochiba
Corp., Japan). Jpn. Kokai Tokkyo Koho JF 2008191499 A 20080821, 44pp.
(Japanese). CODEN: JKXXAF. APPLICATION: JF 2007-27120 20070206.

The optical material is represented by  $\Phi$ - $\Psi$ -A [A = (un)substituted 5(4H)-oxazolon-4-ylidene=methyl, 5(4H)-thiazolon-4-ylidene=methyl, 5(4H)-imidazolon-4-ylidene=methyl, 2(3H)-furanon-3-ylidene=methyl, 3-(dicyanomethylene)-1-indanon-2-2(3H)-furanon-3-ylidene=methyl, 3-(dicyanomethylene)-1-indanon-2-ylidene=methyl,
3-(dicyanomethylene)-2,3-dihydro-1,1-dioxidebenzothiophen-2-ylidene=methyl, 3-cyano-2-(dicyanomethylene)-2,4-dihydrofuran-4-yl,
1-(dicyanomethylene)inden-3-yl, 2-(tricyanovinyl)-5-thienyl,
2-(7,8,8-tricyanoquinodimethan-7-yl)-5-thienyl,
5-(tricyanovinyl)-2,2'-bithiophen-5'-yl,
5-(7,8,8-tricyanoquinodimethan-7-yl)-2,2'-bithiophen-5'-yl; •
(un)substituted 3-alkyl-2(3H)-benzothiazolylidene=methyl,
1,3-dilkyl-1,3-dihydro-2-benzoimidazolylidene=methyl,
1,3-dilkyl-1,3-dihydro-2-benzoimidazolylidene=methyl,
1-alkyl-2(3H)-indolylidene=methyl, 1-alkyl-2(1H)-pyridinylidene=methyl,
1-alkyl-2(1H)-quinolinylidene=methyl, 1-alkyl-2(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-3(1H)-quinolinylidene=methyl,
1-alkyl-3(1H)-quinolinylidene=methyl,
1-alkyl-4(1H)-quinolinylidene=methyl,
1-alkyl-3(1H)-quinolinylidene=methyl,
1-alkyl-3(1H)-quino polymer film, and heating the polymer film at a secondary temperature higher than the primary temperature for poling. The optical modulator has a nonlinear optical

optical
region made of a nonlinear optical polymer film, a pair of electrodes
sandwiching the region, a light injector to the region, and a light
receiver for the light emitted from the region, wherein the polymer film
contains a base polymer and the above nonlinear optical material. The
nonlinear optical material shows high heat resistance.

11 1045854-34-99
RL: IMF (Industrial manufacture); TEM (Technical or engineered material
use); PREF (Preparation); USES (Uses)
(organic nonlinear optical material of N-containing heterocyclic
compound for

L43 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

L43 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

formation of nonlinear optical polymer film used in optical modulator)

RN 1045854-34-9 CAPLUS

CN Propanedinitrile, 2-[3-cyano-4-[7-(1-ethyl-4(1H)-pyridinylidene)-1,3,5-heptatrien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

ANSWER 9 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 8:423751 Document No. 150:504049 Geometry and bond-length alternation in nonlinear optical materials. II. Effects of donor strength in two push-pull molecules. Gainsford, Graeme J.; Bhuiyan, M. Delower H.; Kay, Andrew J. (Industrial Research Limited, Lower Hutt, 31-310, N. Z.). Acta Crystallographica, Section C: Crystal Structure Communications, C64(4), o195-o198 (English) 2008. CODEN: ACSCEE. ISSN: 0108-2701. Publisher: Blackwell Publishing Ltd..

Blackwell Publishing Ltd.

AB The compds.

The compds.

12-(4-cyano-5-dicyanomethylene-2,2-dimethyl-2,5-dihydrofuran-3-yl)vinyl]-N-phenylacetamide, C20H16N4O2,(I), and 2-(3-cyano-5,5-dimethyl-4-[2-(pipreidin-1-yl)vinyl]-2,5-dihydrofuran-2-ylidenelmalononitrile 0.376-hydrate, C17H18N4O·0.376H2O, (II), are novel push-pull mols. Ctystallog, data are given. The significant bonding changes in the polyene chain compared with the parent mol. 2-dicyanomethylene-4,5,5-trimethyl-2,5-dihyrofuran-3-carbonitrile are consistent with the relative electron-donating properties of the acetanilido and piperidine groups. The packing of (I) uses one phenyl-cyano C-H···N and two phenyl-carbonyl C-H···O H bonds. (II) crystallizes with a partial H2O mol. (0.376H2O), consistent with cell packing that is dominated by attractive C-H···N(cyano) interactions. These compds. are precursors to novel nonlinear optical chromophores, studied to

assess the impact of donor strength and the extent of conjugation on bond-length alternation, crystal packing and aggregation. 1149054-01-2 RL: PRP (Properties)

AL: PKF (Properties)
 (orystal structure of)
149054-01-2 CAPUS
Propanedinitrile, 2=[3-cyano-5,5-dimethyl-4-[(1E)-2-(1-piperidinyl)ethenyl]-2(5H)-furanylidene]-, hydrate (50:19) (CA INDEX NAME)

Double bond geometry as shown.

●19/50 H<sub>2</sub>O

L43 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CAPLUS

1026/74-63-3 CAPLOS Benzenesulfonic acid, 4-methyl-, compd. with 2-[3-cyano-5,5-dimethyl-4+[2-[1-methyl-5-(1-piperidinyl)-1H-pyrrol-2-yl]ethenyl]-2(5H)-furanylidene]propanedinitrile, ion(1-) (1:1) (CA I NAME)

CM 1

CRN 1026774-82-2 CMF C22 H23 N5 O

CRN 16722-51-3 CMF C7 H7 O3 S

L43 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2008:420767 Document No. 148:562620 Synthesis and properties of novel
second-order NLO chromophores containing pyrrole as an auxiliary electron
donor. Ma, Xiaohua; Liang, Ran; Yang, Fan; Zhao, Zhenhua; Zhang, Aixin;
Song, Naiheng; Zhou, Qifeng; Zhang, Jianping (Beijing National Laboratory
for Molecular Sciences, Key Laboratory of Polymer Chemistry and Physics

Ministry of Education, Department of Polymer Science and Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, Peop. Rep. China). Journal of Materials Chemistry, 18(15), 1756-1764 (English) 2008. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry. A novel series of second-order NLO chromophores containing pyrrole as an auxiliary electron donor was synthesized via Knoevenagel reactions seen

between

S-aminated N-methylpyrrole-2-carbaldehydes and different
electron-accepting groups, i.e., malononitrile, picolinium tosylate and
2-dicyanomethylene-3-cyano-4,5,5-trimethyl-2,5-dihydrofuram (TCF). Their
corresponding NLO chromophores containing thiophene in the place of
pyrrole
were also prepared for comparison. The resulting NLO chromophores showed
good solubility in common organic solvents such as CHCl3, THF and DMF,
except for
TTCF containing thiophene and TCF, which is soluble in polar aprotic
solvents but
poorly soluble in less polar solvents. NMR studies of these chromophores
showed that, in comparison with thiophene rings in the same type of NLO
chromophores, pyrrole rings had higher electron d., as evidenced by the
up-field chemical shifts of pyrrole protons. TGA investigations showed

thermal stability of these chromophores in nitrogen with the onset weight loss temps. in the range of 203 to 296  $^{\circ}$ C. Fos. solvatochromism of 10-44 nm from dioxane to chloroform were found for these chromophores,

moderate to very large mol. static hyperpolarizabilities (β0) of 57-1490 + 10-30 esu were revealed by hyper-Rayleigh scattering measurements. For chemical bonding to polymer chains, hydroxyl-containing NLO

oxyl-containing NLO chromophores were also prepared and characterized for their linear and nonlinear optical properties.

1026774-81-1P 1026774-83-3P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and properties of novel second-order NLO chromophores containing

aining
pyrrole as auxiliary electron donor)
1026774-81-1 CAPLUS
Benzenesulfonic acid, 4-methyl-, compd. with
2-[3-cyano-5,5-dimethyl-4-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2(5H)furanylidene]propanedinitrile, ion(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 1026774-80-0 CMF C21 H20 N4 O S

(Continued) L43 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN

ANSWER 11 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 3:285086 Document No. 148:347284 Prediction of an agent's or agents' activity across different cells and tissue types. Theodorescu, Dan; Lee, Jae Kyun (USA). PCT Int. Appl. WO 2008027912 A2 20080306, 124pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR,

BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, II, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MM, MX, MX, NA, NG, NI, NO, NZ, CM, PG, PB, FL, FT, RC, RS, KU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ; RW: AT, BE, BF, LJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, MT, NE, NL, FT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2007-US77022 20070828. PRIORITY: US

PIXXD2. APPLICATION: WO 2007-US77022 20070828. PRIORITY: US
2006-840644P
20060828; US 2006-840834P 20061122.

AB The present invention relates to a novel algorithm that uses mol. profile signatures to extrapolate the physiol. processes of one type of cell set (e.g., cell line, tissue, normal or diseased) to predict the activity of an agent or agents against another type of cell set that has never been exposed to the agent in question (drug efficacy prediction). The novel algorithm also allows one to predict the therapeutic response of a patient

algorithm also allows one to promote the patient (or patients) may have to a therapeutic regimen even though the patient (or patients) may have never been exposed to that agent before, thereby allowing for selecting a therapeutic agent or combination of agents that would best suit the patient (i.e., personalized medicine). The present invention also

relates

to methods of using the agents identified by the novel algorithm to treat
a variety of diseases, including cancer.

IT 171082-39-6, NSC 686342
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(prediction of an agent's or agents' activity across different cells
and tissue types for treatment of diseases such as cancer)
RN 171082-39-6 CAPLUS
CN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[2-(4-pyridinyl)ethenyl]-2(5H)furanylidene]- (CA INDEX NAME)

ANSWER 13 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:828339 Document No. 147:364975 Predicting nonlinear optical properties in push-pull molecules based on methyl pyridinium donor and 3-cyano-5,5-dimethyl-2(5H)-furanylidene-propanedinitrile acceptor units using vibrational spectroscopy and density functional theory. McGoverin, Cushla M.; Walsh, Timothy J.; Gordon, Reith C.; Kay, Andrew J.;
 Woolhouse, Anthony D. (Department of Chemistry, MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Otago, Dunedin, N. Z.). Chemical Physics Letters, 443(4-6), 298-303 (English) 2007. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier B.V.
 AB The exptl. Raman, electronic absorption and hyperpolarizability (β 0) data are compared to the calculated parameters for three potential nonlinear

data are compared to the balance...
nonlinear
optical materials based on Me pyridinium donor and
3-cyano-5,5-dimethyl-2(5H)-furanylidene-propanedinitrile acceptor units
linked by a m-chain of 3, 5 and 7 carbon atoms. Using a B3LYP
functional with the 6-31G(d) basis set we obtain predictions of the
f0 values within 20% of those observed in experiment The inclusion of
solvent in the calcus, does not improve the prediction - indeed it

mes worse. This poorer performance is also reflected in the poorer correlation between calculated and exptl. Raman spectra and electronic absorption spectra. 814264-61-8 814264-62-5 814264-63-6 RL: PRP (Properties) (predicting nonlinear optical properties in push-pull mols. based on

IT

pyridinium donor and 3-cyano-5,5-dimethyl-2(5H)-furanylidene-propanedinitrile acceptor units using vibrational spectroscopy and d.

functional theory)
814264-61-4 CAPLUS
Propanedintrile, 2-[3-cyano-5,5-dimethyl-4-[3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene)- (CA INDEX NAME)

Ме

RN

814264-62-5 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[5-(1-methyl-4(1H)-pyridinylidene)-1,3-pentadien-1-y1]-2(5H)-furanylidene)- (CA INDEX NAME)

L43 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 2008:148957 Document No. 150:1803140 2-(3-Cyano-5, 5-dimeth)1-4-f[-4-(piperidin-1-y1)buta-1,3-dienyl]-2,5-dihydrofuran-2-ylidene}malononitrile. Gainsford, Graeme J.; Bhuiyan, M. Delower H.; Kay, Andrew J.; Spek, Anthony L. (Industrial Research

dihydrofuran-2-ylidene|malonontrile. Gainston, Clindustrial Research
Limited,
Lower Hutt, N. Z.). Acta Crystallographica, Section E: Structure Reports
Online, E64(2), c503, c503/1-c503/11 (English) 2008. CODEN: ACSEBH.
ISSN: 1600-5368. URL:
http://journals.iucr.org/e/issues/2008/02/00/qg3141
/gg3141.pdf CTHER SOURCES: CASREACT 150:180314. Publisher: Blackwell
Publishing Ltd.
AB 2-(3-Cyano-5,5-dimethyl-4-[4-(piperidin-1-y1) buta-1,3-dienyl]-2,5dihydrofuran-2-ylidene|malononitrile, C19H20N40, crystallizes as twinned
crystals containing 2 independent mols. which pack into a 3-dimensional
matrix
via several C-H···N(cyano) interactions, with
C···N ranging 3.324(8)-3.568(8) Å and
C-H···N angles of 147-166°. Crystallog. data
are given.
IT 1105024-87-00
RL: PRP (Properties); SFN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)
RN 1105024-87-0 CAPLUS
N Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-4-(1-piperidinyl)-1,3butadien-1-y1]-2(5H)-furanylidene]- (CA INDEX NAME)
Double bond geometry as shown.

Double bond geometry as shown.

L43 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

814264-63-6 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[7-(1-methyl-4(1H)-pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

L43 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2006:427381 Document No. 145:1127650 Antiparallel-Aligned
Neutral-Ground-State and Zwiterionic Chromophores as a Nonlinear Optical
Material. Liao, Yi; Bhattacharjee, Sanchali; Firestone, Kimberly A.;
Eichinger, Bruce E.; Paranji, Rajany Anderson, Cytus A.; Robinson, Bruce
H.; Reid, Philip J.; Dalton, Larry R. (Department of Chemistry,
University H.; Reid, Philip J.; Dalton, Larry .....
University
of Washington, Seattle, WA, 98195, USA). Journal of the American

of Washington, Seattle, WA, 99195, USA). Journal of the American ideal Society, 128(21), 6847-6853 (English) 2006. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 145:112765. Publisher: American Chemical Society. Efficient noncentrosym. arrangement of nonlinear optical (NLO) chromophores with high 1st-order hyperpolarizability ( $\beta$ ) for increased electrooptical (EO) efficiency proved challenging as strong dipolar interactions between the chromophores encourage antiparallel alignment, attenuating the macroscopic EO effect. This work explores a novel approach to simultaneously achieve large  $\beta$  values while providing an adjustable dipole moment by linking a strong neutral-ground-state (NGS) NLO chromophore with pos.  $\beta$  to a zwitterionic (ZMI) chromophore with neg.  $\beta$  in an antiparallel fashion. Probably the overall  $\beta$  of such a structure will should be the sum of the absolute values of the two types of chromophores while the dipole moment will be the difference. Mols. 1-3 were synthesized to test the feasibility of this approach. Mol. dynamics calcus. and NMR data supported that the NGS chromophore component and the ZMI chromophore component self-assemble to an antiparallel conformation in CHC13.

showed that the dipole moment of 1 is close to the difference of the two component chromophores. Hyper-Rayleigh scattering (HRS) studies

component enromopholes. Myper  $m_1 = m_2 = m_3$  confirmed that the 1st hyperpolarizability of 1 is close to the sum of the two component chromophores. These results support the idea that an antiparallel-aligned neutral-ground-state chromophore and a zwitterionic chromophore can simultaneously achieve an increase in  $\beta$  and a decrease of the dipole moment.

895551-99-2P RL: PRP (Prop 551-99-2P
PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(antiparallel-aligned neutral-ground-state and zwitterionic chromophores as a nonlinear optical material)

chromophores as a nonlinear optical material) 895551-99-2 CAPLUS  $\beta$ -Alanine, N-[4-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-fuzanyl]ethenyl]phenyl]-N-methyl-, 2-[4,5-dihydro-4-[(1-methyl-4-(1H)-pyridinylidene)ethylidene]-5-oxo-3-propyl-1H-pyrazol-1-yl]ethyl ester (9CI) (CA INDEX NAME)

L43 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 2006:253983 Document No. 145:513687 The effects of molecular aggregation

isomerization on the fluorescence of "push-pull" hyperpolarizable chromophores. Smith, Gerald J.; Dunford, Cara L.; Kay, Andrew J.; Woolhouse, Anthony D. (Industrial Research Ltd., Lower Hutt, 31310, N. Z.). Journal of Photocholomistry and Photobiology, A: Chemistry, 179(3), 237-242 (English) 2006. CODEN: JPPCEJ. ISSN: 1010-6030. Publisher: Elsevier B.V.

AB Hyperpolarizable organic mols. are attracting interest for use in nonlinear optical devices. Some zwitterionic merocyanine chromophores with exceptionally high first hyperpolarizabilities have been synthesized that possess an electron donor molety coupled to an electron acceptor through a

conjugated double bond system. Aligned arrays of these mols. tethered to a polyurethane backbone and spun onto a substrate to form a thin film, respond to the application of external elec. fields with changes to their refractive indexes, i.e. the electro-optic effect. This behavior can be capitalized upon to fabricate optical switches and modulators. High concess, or loadings, of these nonlinear optical mols. in thin films are required to produce a usable electro-optic effect, ca. 0.1-0.5 mol L-1, and this promotes mol. aggregation which alters their polarizabilities

also has implications for their photostabilities. The fluorescence spectra of these mols. in polymer films at ambient temperature and in

solution in a 9:1 ethanol-water mixture over a range of temps. down to 80 K show a substantial blue shift as the temperature is lowered. This is

attributed to a reduction in the solvating power of the solvent as it becomes

noreasingly
more viscous at lower temps. At the lowest temps, studied a shoulder on
the lower energy side of the fluorescence spectral distribution is
apparent which is ascribed to the formation of antiparallel
dimers/aggregates; a consequence of the highly dipolar character of these
mols. In addition, dual fluorescence is observed in high viscosity
environments character of these

omments suggesting the involvement of twisting about the bridging conjugated bond system that links the electron donor to the electron acceptor. 814264-64-7

RL: PRP (Properties); TEM (Technical or engineered material use); USES

(Uses)
(effects of mol. aggregation and isomerization on fluorescence of push-pull hyperpolarizable chromophores)
814264-64-7 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[3-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CIRDEX NAME)

L43 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

L43 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSWER 16 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 5:1322081 Document No. 145:3787400 Synthesis of a new series of 'RHS' chromophores and NLO polymers. Beaudin, Andrew M. R.; Kay, Andrew J.; Woolhouse, Anthony D. (Opto-Organics Group, Industrial Research Ltd., Lower Butt, N. Z.). Proceedings of SPIE-The International Society for Optical Engineering, 5971(Photonic Applications in Nonlinear Optics, Nanophotonics and Microwave Photonics), 597101/1-597101/10 (English) 5.

2005

. CODEN: PSISDG. ISSN: 0277-786X. OTHER SOURCES: CASREACT 145:378740. Publisher: SPIE-The International Society for Optical Engineering. A series of right-hand-side (RRS) hydroxy functionalized merocyanines containing a powerful cyanodicyanomethylidenedihydrofuran electron

Peptor

has been designed and synthesized. Using the "build up" approach to synthesis, variations in both the donor moiety and conjugation length of these zwitterionic systems are possible, thereby giving rise to a suite

chromophores. Hyper-Raleigh scattering has confirmed that the highly conjugated chromophores have large first hyperpolarizabilities (β0) - values that are of a similar magnitude to many of those reported for "bench mark" left-hand-side systems. The hydroxy functionalized chromophores were successfully grafted at various loadings onto a series of recently developed carboxylic acid containing polyetherimides.

814264-64-7P 814264-65-8P 910999-68-7P 910999-68-9P 910999-0-91P RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (chromophore; synthesis and characterization of right-hand-side chromophores and NLO polyimides containing them)
814264-64-7 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[3-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(SH)-furanylidene]- (CA INDEX NAME)

 $814264-65-8 \quad CAPLUS \\ Propaned in itrile, \quad 2-[3-cyano-4-[5-[1-(2,3-dihydroxypropy1)-4(1H)-pyridinylidene]-1,3-pentadien-1-y1]-5,5-dimethyl-2(5H)-furanylidene]-1,3-pentadien-1-y1]-5,5-dimethyl-2(5H)-furanylidene]-1,3-pentadien-1-y1]-5,5-dimethyl-2(5H)-furanylidene]-1,3-pentadien-1-y1]-1,5-dimethyl-2(5H)-1,3-pentadien-1-y1]-1,5-dimethyl-2(5H)-1,5-di$ 

INDEX NAME)

L43 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L43 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

910999-68-7 CAPLUS Propanedinitrile, 2-[3-cyano-4-[3-[1-(2-hydroxyethy1)-4(1H)-pyridinylidene]-1-propen-1-y1]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

RN CN

910999-69-8 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[5-[1-(2-hydroxyethyl)-4(1H)-pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-

INDEX NAME)

910999-70-1 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[7-[1-(2-hydroxyethy1)-4(1H)-pyridinylidene]-1,3,5-heptatrien-1-y1]-5,5-dimethy1-2(5H)-furanylidene]-(CA INDEX NAME)

L43 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2005:34510 Document No. 142:1160140 Fluorophore compounds and their use in
labeling biomolecules and biological structures. Moerner, William E.;
Twieg, Robert J.; Kline, Douglas W.; He, Meng (Stanford University,

. U.S. Pat. Appl. Publ. US 20050003109 Al 20050113, 44 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-604282 20030708. Fluorophore compds. and methods for their use are disclosed. The fluorophores contain a 2-dicyanomethylen-3-cyano-2,5-dihydrofuran (DCDHF) molety and one or more donor groups conjugated to the 2-dicyanomethylen-3-cyano-2,5-dihydrofuran group (e.g.,

3-cyano-2-dicyanomethylen-4-[4-(N,N-dihexylaminophenyl)]-5,5-dimethyl-2,5-dihydrofuran, DCDHF-6). The donor groups can contain atoms with free electron pairs such as oxygen, sulfur, nitrogen, or phosphorous. The fluorophore compds. can be used to label and detect biol. mols. and biol. structures either in vivo or in vitro.

IT 821789-34-8P, 3-Cyano-2-dicyanomethylen-5,5-dimethyl-4-[4-(3,5-dimethylpiperidin-1-ylphenyl]-2,5-dihydrofuran RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); RIO.

BIOL

(Biological study); PREP (Preparation); USES (Uses)
(preparation of fluorophore compds. containing
2-dicyanomethylen-3-cyano-2,5-dihydrofuran for labeling biomols.)
RN 821789-34-8 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[4-4],5-dimethyl-1-piperidinyl)phenyl]-5,5dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L43 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
2004:1127374 Document No. 142:745550 A preparation of zwitterionic
non-linear [(pyridinylidenealkylene)furanylidene]propanedinitrile
derivatives, useful as optical chromophores (optophores). Woolhouse,
Anthony David; Kay, Andrew John (Industrial Research Limited, N. Z.).
PCT

Int. Appl. WO 2004111043 A1 20041223, 47 pp. DESIGNATED STATES: W. AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, DI, III, III, K, FR, KE, KG, KF, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ, NA, NI, NO, NZ, CM, PG, PH, PI, PT, BO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, RW; AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, MI, MR, NE, NL, FT, SI, SN, TD, FRIORITY: NZ 2003-526561 20030618.

AB The invention relates to a preparation of zwitterionic second order non-linear

linear optophores of formula I [wherein: L is a linking group comprising (un)substituted chain of 3,5, or 7 carbon atoms which, together with the double bond linking D to L forms a conjugated polyenic chain, R1 and R2 are independently selected from alkyl, hydroxyalkyl, or p-C6H4-OAc; D is

a heterocycle]. These optophores display a large and efficient non-linear optical response and therefore can be used in the production of optoelectronic devices. For instance, (furanylidene)propanedinitrile derivative II (electronic absorption data in DMF: \text{\mathcal{L}} \text{\mathcal{L}} = 570 nm, log10e = 4.86) was prepared with a yield of 38%.

IT 814264-61-4P 814264-62-5P 814264-63-6P 814264-63-6P 814264-63-6P 814264-66-9P 814264-66-9P 814264-66-PB 814264-66-9P

ANSWER 18 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) Propanedinitrile, 2-[3-cyano-4-[3-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

814264-65-8 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[5-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-CN

(CA INDEX NAME)

814264-66-9 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[3-(1-methyl-2(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

814264-67-0 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[5-(1-methyl-2(1H)-pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

L43 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 814264-70-5P (Continued) 814264-70-5p
RL: IMF (Industrial manufacture); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of [(pyridiny)1idenealkylene)furanylidene]propanedinitrile derive. useful as optophores)
814264-61-4 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

814264-62-5 CAPLUS Propandintrile, 2-[3-cyano-5,5-dimethyl-4-[5-(1-methyl-4(1H)-pyridinylldene)-1,3-pentadien-1-yl]-2(5H)-furanylldene)- (CA INDEX NAME)

814264-63-6 CAPLUS Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[7-(1-methyl-4(1H)-pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]- (CNAME) (CA INDEX

RN 814264-64-7 CAPLUS

L43 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

814264-68-1 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[7-(1-methyl-2(1H)-pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

814264-69-2 CAPLUS
Propanedinitrile, 2-{3-cyano-4-{3-{1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene}-1-propen-1-yl}-5,5-dimethyl-2(5H)-furanylidene}- (CA INDEX NRME)

814264-70-5 CAPLUS
Proparedinitrile, 2-[3-cyano-4-[5-[1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-

L43 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L43 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

712273-74-0 CAPLUS
PropanedInitrile, 2-[4-[(1E)-3-[1-[2-(acetyloxy)ethyl]-4(1H)pyridinyllidene]-1-propen-1-yl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene](CA INDEX NAME)

Double bond geometry as shown.

712273-75-1 CAPLUS

Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-5-(1-methyl-4(1H)-pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene)- (CA INDEX NAM

Double bond geometry as shown.

712273-76-2 CAPLUS
Propanedinitrile,
-cyano-5,5-dimethyl-4-[(1E,3E,5E)-7-(1-methyl-4(1H)pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L43 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN 2004;283941 Document No. 141;729550 Synthesis and linear/nonlinear optical properties of a new class of 'RHS' NLO chromophore. Kay, Andrew J.; Woolhouse, Anthony D.; Zhao, Yuxia; Clays, Koen (Opto-Organics Group, Industrial Research Limited, Lower Hutt, N. Z.). Journal of Materials Chemistry, 14(8), 1321-1330 (English) 2004. CODEN: WMACEP. ISSN: 0959-9428. OTHER SOURCES: CASREACT 141:72955. Publisher: Royal Society of Chemistry.

0959-9428. OTHER SOURCES: CASKERGI 1411/2237. FURTISHER. DEPT. CONTROLL OF CHEMISTRY.
Examples of a new class of zwitterionic, "right-hand side" (RHS)
merocyanines containing a cyanodicyanomethylidenedihydrofuran electron
acceptor were prepared As well as allowing for the facile synthesis of
these chromophores, the synthetic methodol. enables considerable

variation in both the donor moiety as well as the extent of conjugation between the donor and acceptor systems. As expected, all of these RHS systems are neg. solvatochromic, with the difference between  $\lambda max (polar vs. nonpolar solvents) increasing with the extent of conjugation. In accord with expectations, hyper-Raleigh scattering (HRS) measurements confirm that mols. with the greatest conjugation pathway have the largest first hyperpolarizabilities, <math display="inline">\beta o$ . In addition, the HRS evaluation indicates that the 4-quinolinylidene donor nucleus is superior to both the 4-pyridinylidene and benzothiazolylidene systems. The figures of merit,  $\mu(\text{calc}).\beta o(\text{measured})$ , that are obtained for some of these compds., are of a similar magnitude to the best "left hand side" examples reported in the literature. To demonstrate the versatility of the synthetic technique, representative polymer-tetherable derivs. of these compds.

prepared, as have the corresponding TDI-based polyurethanes.

712273-71-7P 712273-72-8P 712273-74-0P
712273-75-1P 712273-76-2P 712273-77-3P
712273-63-3P 712273-66-4P 712273-87-3P
712273-68-6P 712273-89-7P
RL: FRP (Properties); SFN (Synthetic preparation); PREP (Preparation)
(synthesis and linear/nonlinear optical properties of new class of right-hand-side NLO chromophore)
712273-71-7 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene)- (CA INDEX NAME)

Double bond geometry as shown.

712273-72-8 CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E)-3-[1-(2,3-dihydroxypropy1)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L43 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

712273-77-3 CAPLUS Propanedinitrile,  $2-[3-{\rm cyano}-4-[(1E,3E)-5-[1-(2,3-{\rm dihydroxypropy1})-4(1H)-pyridinylidene]-1,3-pentadien-1-y1]-5,5-dimethy1-2(5H)-furanylidene]-$ 

INDEX NAME)

Double bond geometry as shown.

712273-85-3 CAPLUS Fropanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E)-4-(1-methyl-2(1H)-pyridinylidene)-2-buten-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

712273-86-4 CAPLUS
Propanedinitrile,
-cyano-5,5-dimethyl-4-[(2E,4E,6E)-6-(1-methyl-2(1H)pyridinylidene)-2,4-hexadien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L43 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

712273-87-5 CAPLUS Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E,8E)-8-(1-methyl-2(1H)-pyridinylidene)-2,4,6-octatrien-1-yl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 712273-88-6 CAPLUS
CN Propanedinitrile, 2-[3-cyano-4-[(2E,4E)-4-[1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene]-2-buten-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX

NAME)

L43 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Double bond geometry as shown.

712273-89-7 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(2E,4E,6E)-6-[1-(2,3-dihydroxypropy1)-

2(1H)-pyridinylidene]-2,4-hexadien-1-y1]-5,5-dimethyl-2(5H)-furanylidene]-(CA INDEX NAME)

Double bond geometry as shown.

143 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN
1995:752764 Document No. 124:85310 Original Reference No. 124:1805a,1808a
Synthesis of substituted dicyanomethylendihydrofurans. Melikian, Gaguik;
Rouessac, Francis P.; Alexandre, Christian (Laboratoire de Synthese
Organique, Faculte des Sciences, Le Mans, 72017, Fr.). Synthetic
Communications, 25(19), 3045-51 (Rnglish) 1995. CODEN: SYNCAV. ISSN:
0039-7911. OTHER SOURCES: CASRRACT 124:8531. Publisher: Dekker.
AB A simple and efficient method for the preparation of the title compds. is
described from α-ketols and malonomitrile in the presence of sodium
ethylate at room temperature These compds. lead to unsatd. derivs. by
condensation with aldehydes. For example, condensation reaction of
propanedinitrile and 3-hydroxy-3-methyl-2-butanone gave
(3-cyano-2,5-dihydro-4,5-trimethyl-2-furanylidene)propanedinitrile.
IT 171082-37-4P 171082-38-5P 171082-39-6P
RL: SPN (Synthetic preparation); PRPF (Preparation)
(preparation of dicyanomethylendihydrofurans from hydroxy ketones and
propanedinitrile)
RN 171082-37-4 CAPLUS
CN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[2-(2-pyridinyl)ethenyl]-2(5H)furanylidene]- (CA INDEX NAME)

RN 171082-38-5 CAPLUS CN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(3-pyridinyl)ethenyl]-2(5H)-furanylidene]- (CA INDEX NAME)

RN 171082-39-6 CAPLUS CN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(4-pyridinyl)ethenyl]-2(5H)-furanylidene]- (CA INDEX NAME)

L43 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L11

L12

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=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
    FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
               STRUCTURE UPLOADED
L1
             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
L10
             0 S L3 AND L9
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26 S ELECTRO-OPTIC CHROMOPHORES

12 S L4 OR L9

L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37 L38		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41 L42	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL 54 S L41 AND C5N/RF
L43	FILE	'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010 20 S L42

2049 C2NS/RF

=> s 141 and Se/els 195781 SE/ELS

L48 0 L41 AND SE/ELS

=> s 141 and Se/es 0 SE/ES

L49 0 L41 AND SE/ES

=> s 141 and c2no/rf 470 C2NO/RF L50 0 L41 AND C2NO/RF

This file contains CAS Registry Numbers for easy and accurate substance identification.

# => d his

L4

L8

(FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 11 S L3

FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010

FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5 TRA L4 1- RN : 172 TERMS

FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 L6 172 SEA L5

L7 1 S L3 NOT L6

FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 0 S OTOPHORE

L27 L28	FILE	'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 6 S L25 AND 5<=REF.CAPLUS 19 S L25 NOT L27
L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL

L51 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 2010:304297 Document No. 152:556918 Toward highly efficient NLO chromophores: Synthesis and properties of heterocycle-based

chromophores: Synthesis and properties of heterocycle-based electronically gradient dipolar NLO chromophores: Ma, Xiaohua; Ma, Fei; Zhao, Zhenhua; Song, Naiheng; Zhang, Jianping (Beijing National Laboratory for Molecular Sciences, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Department of Polymer Science and Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, Peop. Rep. China). Journal of Materials Chemistry, 20(12), 2369-2380 (English) 2010. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB To realize organic nonlinear optical (NLO) chromophores with optimized ground-state polarization and very large mol. optical nonlinearities, a novel series of heterocycle-based electronically gradient dipolar chromophores were designed and synthesized. These chromophores are featured by their same strong electron acceptor (i.e., 2-dioyanomethylene-3-cyano-4, 5,5-trimethyl-2,5-dihydrofuran, TCF) and the same length of x-conjugation, but different electron donors (e.g., dialkylamine and dianisylamine), different (heterolarons. with varying electron densities (i.e., pyrrole, thiophene, and benzene) as the auxiliary donor, and electron-poor 1, 3-heteroarom. thiazole with different

auxiliary donor, and electron poor C2, "matched", or electron-poor C2, "un-matched", or electron-rich C5, "un-matched", is connected to the acceptor) as the auxiliary acceptor, which allows for a systematic fine-tuning of the ground-state polarization. The gradient electronic structures and

mal properties of these NLO chromophores were carefully characterized by IH NMR, CV, UV-vis, and Hyper-Rayleigh scattering expts. All the NLO chromophores exhibited very large static mol. first hyperpolarizabilities ( $\beta$ 0) in the range of 450-960 + 10-30 esu, which showed significant dependence on the gradient electronic structures. Upon using electron-rich heteroarom. cycle as the auxiliary donor, "matched" zole

RL: PEP (Physical, engineering or chemical process); PRP (Properties);

SPN

(Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PRCC (Process); USES (Uses) (toward highly efficient NLO chromophores and synthesis and properties of heterocycle-based electronically gradient dipolar NLO chromophores) 1225601-89-7 CAPLUS Propanedinitrinie, 2=[3-cyano-4-[(1E)-2-[2-[(1E)-2-[4-(dimethylamino)phenyl]ethenyl]-5-thiazolyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) methoxyphenyl)aminophenyl]ethenyl]-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

1225601-96-6 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(4-methoxyphenyl)amino]phenyl]ethenyl]-2-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

1225601-98-8 CAPLUS Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[4-[(1E)-2-[5-(1-

piperidiny1) -2-thieny1]etheny1]-2-thiazoly1]etheny1]-2(5H)-furanylidene](CA INDEX NAME)

Double bond geometry as shown.

L51 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Double bond geometry as shown.

RN 1225601-90-0 CAPLUS
CN Propanedinitrile,
2-[3-cyano-5,5-dimethy1-4-[(1E)-2-[2-[(1E)-2-[1-methy1-5(1-piperidiny1)-1H-pyrrol-2-y1]etheny1]-5-thiazoly1]etheny1]-2(5H)furanylidene]- (CA INDEX NAME)

Double bond geometry as shown

1225601-91-1 CAPLUS Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[2-[(1E)-2-[5-(1-10-2-[3-10-2

piperidiny1) -2-thieny1]etheny1]-5-thiazoly1]etheny1]-2(5H)-furanylidene](CA INDEX NAME)

Double bond geometry as shown.

1225601-94-4 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[2-[(1E)-2-[4-[bis(4-

L51 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSMER 2 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 9:365685 Document No. 150:4594270 Modulated Conjugation as a Means of Improving the Intrinsic Hyperpolarizability. Perez-Moreno, Javier; Zhao, Yuxia; Clays, Koen, Kuzyk, Mark G.; Shen, Yuquan, Qiu, Ling; Hao, Jumin; Guo, Kunpeng (Department of Chemistry, University of Leuven, Louvain, B-3001, Belg.). Journal of the American Chemical Society, 131(14), 5084-5093 (English) 2009. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 150:459427. Publisher: American Chemical Society. A new strategy for optimizing the 1st hyperpolarizability based on the concept of a modulated conjugated path in linear mols. was studied.

Seven
novel chromophores with different types of conjugated paths were
synthesized and characterized. Hyper-Rayleigh scattering expts.

confirmed
that modulated conjugation paths that include benzene, thiophene, and/or
thiazole rings in combination with azo and/or ethenyl linkages between
dihydroxyethylamino donor groups and various acceptor groups result in
enhanced intrinsic hyperpolarizabilities that exceed the long-standing
apparent limit for two of the chromophores. The exptl. results are
analyzed and interpreted in the context of quantum limits, which show
that

conjugation modulation of the bridge in donor/acceptor mols. simultaneously optimizes the transition moments and the energy-level spacing. 716378-72-2P RL: FRP (Properties); SFN (Synthetic preparation); PREP (Preparation) (modulated conjugation as means of improving intrinsic hyperpolarizability) 716378-72-2 CAPLUS
Propanedinitrile, 2-[4-[2-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 2008:415128 Document No. 149:79068 Order of magnitude effects of thiazole regioisomerism on the near-IR two-photon cross-sections of dipolar chromophores. Schmidt, Karin; Leclercq, Amalia; Zojer, Egbert; Lawson, PaDreyia V.; Jang, Sei-Hum; Barlow, Stephen; Jen, Alex K.-Y.; Marder,

R:, Bredas, Jean-Luc (School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, GA, 30332-0400, USA). Advanced Functional Materials, 18(5), 794-801 (English) 2008. CODEN. AFMDC6. ISSN: 1616-301X. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.
We have investigated computationally the two-photon absorption (2PA) properties of donor-acceptor dipolar chromophores, the conjugated backbones of which contain two five-membered heterocyclic groups which

be electron-rich (thiophene-2,5-diyl) and/or electron-deficient (thiazole-2,5-diyl). Quantum-chemical calcns. (INDO/MRDCI/S-tensor and Sum-Over-States calcns. based on DFT-optimized geometries) indicate that the two-photon cross-sections into the lowest two excited states S1 and

can be tuned by more than an order of magnitude by varying the nature, order, and, in the case of thiazole, orientation of the heterocycles. Going from one thiazole regioisomer to the other has the strongest impact on the 2PA spectra and can even invert the ratio between the 2PA cross-sections of Sl and S2. An essential-state anal. reveals that different channels dominate 2PA into Sl and S2. The sensitivity of 2PA into Sl towards the orientation of the thiazole ring stems from a local modulation on the thiazole ring of the change in state dipole moment upon excitation to Sl, AµOl, whereas the dominant essential parameter through which the thiazole orientation affects 2PA into S2 is the transition dipole moment between Sl and S2, µl2. 1034158-73-0 1034158-73-9 1034158-73-0 1034158-73-0 RL: PRP (Properties)

1034158-74-1 1034158-75-2 1034158-76-5
RL: PRP (Properties)
(order of magnitude effects of thiazole regioisomerism on near-IR
two-photon cross-sections of dipolar chromophores)
1034158-71-8 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-butylphenyl]-2-thienyl]-thenyl]-2-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

1034158-72-9 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[2-[(1E)-2-[5-[(1E)-2-(4-butylphenyl)-thenyl]-2-thienyl]ethenyl]-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

1034158-73-0 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-(4-butyl)phenyl)]-2-thiazolyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

1034158-74-1 CAPLUS
Propanedinitrile, 2=[4-[(1E)-2-[5-[(1E)-2-[2-[(1E)-2-(4-butylphenyl)-5-thiazolyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

butylphenyl)ethenyl]-2-thiazolyl]ethenyl]-2-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L51 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

1034158-76-3 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[2-[(1E)-2-[2-[(1E)-2-(4-

butylpheny1)etheny1]-5-thiazoly1]etheny1]-5-thiazoly1]etheny1]-3-cyano-5,5dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L51 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

L51 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
2007:1205147 Document No. 148:365650 Record-high intrinsic
hyperpolarizabilities for polymeric electro-optic modulators.
Perez-Moreno, Javier; Asselberghs, Inge; Zhao, Yuxia; Song, Kai;
Nakanishi, Hachiro; Okada, Shuji; Nogi, Kyoko; Kim, Oh-Ril; Je, Jongtae;
Matrai, Janka; De Maeyer, Marc; Kuzyk, Mark G.; Clays, Koen (Department

of
Chemistry, Univ. of Leuven, Louvain, B-3001, Belg.). Proceedings of
SPIE-The International Society for Optical Engineering,
6713 (Nanophotonics
and Macrophotonics for Space Environments), 671303/1-671303/14 (English)
2007. CODEN: PSISDG. ISSN: 0277-786X. Publisher: SPIE-The

and Macrophotonics for Space Environments), 6/13/03/1-6/13/03/14 (English) 2007. CODEN: PSISDO. ISSN: 0277-786X. Publisher: SPIE-The International Society for Optical Engineering.

AB The results of three independently strategies for the optimizations of electro-optic organic chromophores is presented. The first strategy to enhance the nonlinear optical response, applied at the mol. level, is the extension of the conjugation path in a ionic chromophore. The second strategy, applied at the supramol. level, is the bottom-up nano-engineering of an inclusion complex of the ionic chromophore in an amylose helix. The third strategy, also applied at the mol. level, is to use a modulated conjugation path between donor and acceptor in order to localize eigenfunctions on different parts of the mol. The first hyperpolarizability of the different series of compds. has been exptl. determined by frequency-resolved femtosecond hyper-Rayleigh scattering.

effects of the three different enhancement strategies are analyzed and interpreted in terms of the quantum limits. 716378-72-2 RI: PEP (Physical, engineering or chemical process); PRP (Properties);

C (Process) (record-high intrinsic hyperpolarizabilities for polymeric electro-optic modulators)
716378-72-2 CAPLUS
Propanedinitrile, 2-[4-[2-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
2007:1168150 Document No. 148:295179 Modulated conjugation for record-high
intrinsic hyperpolarisabilities. Perez-Moreno, Javier; Clays, Koen;
Kuzyk, Mark G., Zhao, Yuxie; Shen, Yuquan; Qiu, Ling; Hao, Juming
(Department of Chemistry, Univ. of Leuven, Louvain, B-3001, Belg.).
Proceedings of SPIE-The International Society for Optical Engineering,
6653(Linear and Nonlinear Optics of Organic Materials VII),
66530WJ-166530W/8 (English) 2007. CODEN: PSISD. ISSN. 0277-786X.
Publisher: SPIE-The International Society for Optical Engineering.
AB The effects of a complex hybrid conjugation path in linear mols. as an
strategy to optimize the intrinsic first hyperpolarizability is
investigated. A series of 7 novel chromophores with different hybrid
conjugation paths were synthesized and characterized. Hyper-Rayleigh
scattering expts. confirm that complex hybrid conjugation paths,
including

including
benzene, thiophene and/or thiazole rings in combination with azo- and/or
ethenyl-linkages, between a dihydroxyethylamino donor group and different
acceptor groups, results in an enhanced intrinsic hyperpolarizability

that

exceed the apparent limit for two of the chromophores.

IT 1008099-91-9

RL: PRP (Properties)

(modulated conjugation for record-high intrinsic hyperpolarizabilities)

rpolarizabilities)
1008099-91-9 CAPLUS
Propanedinitrile, 2-[4-[2-[2-[4-[bis(2hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3cyanodihydro-5,5-dimethyl-2(3H)-furanylidenel- (CA INDEX NAME)

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 196107 Document No. 146:379495 Modulated conjugation as a means for attaining a record high intrinsic hyperpolarizability. Perez-Moreno, Javier; Zhao, Yuxia; Clays, Koen; Kuzyk, Mark G. (Department of

Javier; Zhao, Yuxia; Clays, Koen; Kuzyk, Mask G. (Department of Chemistry,
University of Leuven, Louvain, B-3001, Belg.). Optics Letters, 32(1),
59-61 (English) 2007. CODEN: OPLEDP. ISSN: 0146-9592. Publisher:
Optical Society of America.

AB We report on a series of chromophores that have been synthesized with a modulated conjugation path between donor and acceptor. Ryper-Rayleigh scattering measurements of the best mol. show an enhanced intrinsic hyperpolarizability that breaches the apparent limit of all previously studied mols.

IT 930648-59-2
RL: PFP (Properties)
(modulated conjugation as means for attaining high intrinsic hyperpolarizability)
RN 930648-59-2 CAPLUS
Propanedinitriability, 2-[4-[2-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-4,5-dihydro-5-thlazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 2005:1076309 Document No. 144:301132 Frequency-agile hyper-Rayleigh scattering studies of electro-optic chromophores. Firestone, Kimberly

Lao, David B.; Casmier, Daniel M.; Clot, Olivier; Dalton, Larry R.; Reid, Phillip J. (Department of Chemistry, Univ. of Washington, Seattle, WM, 98195-1700, USA). Proceedings of SPIE-The International Society for Optical Engineering, 5935 (Linear and Nonlinear Optics of Organic

Optical Engineering, 5935 (Linear and Nonlinear Optics of Organic Materials

V), 59350P/1-59350P/9 (English) 2005. CODEN: PSISDG. ISSN: 0277-786X.

Publisher: SPIE-The International Society for Optical Engineering.

AB Hyper-Rayleigh scattering (BRS) is used to measure the first-hyperpolarizability (B) of electro-optic (EO) chromophores.

One of the inherent concerns in any HRS measurement is the extent to

resonant enhancement contributes to the observed intensity thereby

leading to lead electro-optical devices. One way to address this concern is to employ increasingly longer excitation wavelengths far from resonance. However, in charge-transfer-based non-linear optical chromophores, enhanced  $\beta$  generally correlates with a red-shift of the charge transfer absorption band so that even at the longest excitation wavelengths generally

employed  $\qquad \text{in HRS studies, resonant enhancement remains an issue.} \ \ \, \text{We have adopted}$ an

alternative approach in which the wavelength dispersion of the  ${\tt HRS}$  intensity is determined by performing measurements at a variety of excitation

vation wavelengths. This approach allows one to ascertain the role of resonance enhancement thereby allowing for more accurate correlation of improved  $\beta$  with mol. architecture. We report the results of our HRS studies for nine chromophores employing excitation wavelengths ranging from 780

1907 nm. Our HRS results demonstrate good agreement with the predictions of d. functional theory. This synthesis of exptl. and theor. techniques has resulted in more effective designs for the next generations of electro-optical chromophores. 873803-00-6 873803-07-7

IT

873803-06-6 873803-07-7
RL: PRP (Properties)
 (frequency-agile hyper-Rayleigh scattering studies of electro-optic chromophores)
873803-06-6 CAPLUS
Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[2-[(1E)-2-[4-(dieth)lamino)phenyl]ethenyl]-5-thiazolyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L51 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 2006:923589 Document No. 146:489939 Modulated conjugation as a means for breaching the apparent limit of the hyperpolarizability. Perez-Moreno Javier; Clays, Koen; Zhao, Yuxia; Kuzyk, Mark G. (Department of Perez-Moreno,

Chemistry, University of Leuven, Louvain, B-3001, Belg.). Los Alamos Natio Laboratory, Preprint Archive, Physics 1-3, arXiv:physics/0608300

(English)

31 Aug 2006. CODEN: LNPHF9. URL:
http://aps.arxiv.org/PS\_cache/physics/pdf/0608/0608300.pdf Publisher:

Alamos National Laboratory.

Chromophores that were synthesized with a modulated conjugation path between donor and acceptor are reported. Byper-Rayleigh scattering measurements of the best mol. shows an enhanced hyperpolarizability that breaches the apparent limit. 716378-72.

REPR (Properties) (modulated conjugation as means for breaching apparent limit of hyperpolarizability of) 716378-72-2 CAPLUS

Propanedinitrile, 2-[4-[2-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4(diethylamino)phenyl]ethenyl]-2-thiazolyl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L51 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN 2005:358523 Document No. 143:777830 Two-Photon Absorption at Telecommunications Wavelengths in a Dipolar Chromophore with a Pyrrole Auxiliary Donor and Thiazole Auxiliary Acceptor. Beverina, Luca; Fu,

Leclercq, Amalia; Zojer, Egbert; Pacher, Peter; Barlow, Stephen; Van Stryland, Eric W.; Hagan, David J.; Bredas, Jean-Luc; Marder, Seth R. (School of Chemistry and Biochemistry, Center for Organic Photonics an Electronics, Georgia Institute of Technology, Atlanta, GA, 30332-0400, USA). Journal of the American Chemical Society, 127(20), 7282-7283 (English) 2005. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT

AGCI 43:77783. Publisher: American Chemical Society.
Three new dipolar chromophores based on a dialkyaminophenyl donor, a pyrrole auxiliary donor, a thiazole auxiliary acceptor, and strong heterocyclic acceptors have been synthesized. For one of these compds.

have measured a very large non-degenerate two-photon cross section of ca. 1500 GM in the near-IR telecommunications range using a pump-probe technique. Calcns. indicate the cross section for degenerate two-photon absorption is likely to be ca. 60% of this value. 855773-97-6P 855774-00-4P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (two-photon absorption at telecommunications wavelengths in a dipolar chromophore with a pyrrole auxiliary donor and thiazole auxiliary acceptor)

acceptor)
855773-97-6 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[2-[2-[5-[2-[4(dibutylamino)phenyl]ethenyl]-1-hexyl-1H-pyrrol-2-yl]ethenyl]-5thiazolyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

855774-00-4 CAPLUS Propanedinitrile, 2-[3-cyano-4-[4-[2-[2-[5-[2-[4-

(dibutylamino)phenyl]ethenyl]-1-hexyl-1H-pyrro1-2-yl]ethenyl]-5-thiazolyl]-1,3-butadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L51 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
2004:211926 Document No. 141:95181 Study on novel second-order NLO
azo-based
chromophores containing strong electron-withdrawing groups and different
conjugated bridges. Qiu, Ling; Shen, Yuquan; Hao, Jumin; Zhai, Jianfeng;
Zu, Fenghua; Zhang, Tao; Zhao, Yuxia; Clays, K.; Persoons, A. (Technical
Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing,
100101, Peop. Rep. China). Journal of Materials Science, 39(7),
2335-2340
(English) 2004. CODEN: JMTSAS. ISSN: 0022-2461. Publisher: Kluwer
Academic Publishers.
AB Novel NLO azo-based chromophores containing strong electron-withdrawing
groups

AB Novel NLO azo-based chromophores containing arrows where synthesized and characterized.  $\beta$  Values were measured by HRS method, they are in the range of 238-1459 + 10-30 esu at the fundamental wavelength of 800 nm. For chromophore 3 and 4,  $\beta$  values at the fundamental wavelength of 106 to 4 nm were also measured, they are 1575 + 10-30 esu and 935 + 10-30 esu, resp. Thermal stabilities for these chromophores are reported. We also discuss the effects of different acceptors and conjugating moleties on  $\beta$ .

IT 716378-72-2P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (second-order NLO azo-based chromophores containing strong

(second-order NLO azo-based chromophores containing strong electron-withdrawing groups and different conjugated bridges) 716378-72-2 CAPLUS Propanedinitrile, 2-[4-[2-[2-[4-[bis(2-

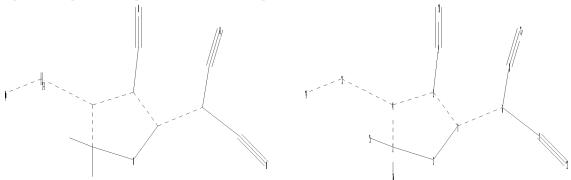
hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

HO-CH2-CH2 HO-CH2-CH2-N

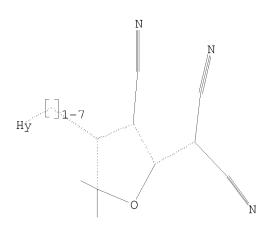
L51 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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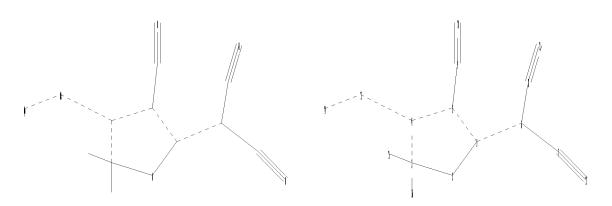


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chain nodes :
6  7  8  9  14
ring nodes :
1  2  3  4  5
ring/chain nodes :
10  11  12  13  15  16
chain bonds :
1-6  3-15  3-16  4-13  5-9  6-7  6-8  7-12  8-11  9-10
ring/chain bonds :
13-14
ring bonds :
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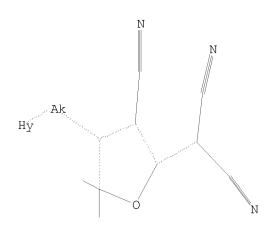


Structure attributes must be viewed using STN Express query preparation.

=> s 152
 REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



```
chain nodes :
6  7  8  9  13  14
ring nodes :
1  2  3  4  5
ring/chain nodes :
10  11  12  15  16
chain bonds :
1-6  3-15  3-16  4-13  5-9  6-7  6-8  7-12  8-11  9-10  13-14
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
1-2  1-5  1-6  2-3  3-4  4-5  4-13  7-12  8-11  9-10  13-14
```



Structure attributes must be viewed using STN Express query preparation.

=> s 153
 REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

STRUCTURE FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4 DICTIONARY FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d his

(FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 14 S L1 FULL

10560670.trn				
L19		TRA L17 1- RN : 3023 TERMS		
L20 L21 L22 L23 L24 L25		'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 214 S L20 AND C5N/RF 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE 25 S L22 OR L23 25 S L24 NOT L3		
L26	FILE	'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25		
	FILE	'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010		
L27 L28		'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 6 S L25 AND 5<=REF.CAPLUS 19 S L25 NOT L27		
L29 L30		'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28		
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL		
	FILE	'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010		

=> s sub=141 sam 153

FILE 'CAPLUS' ENTERED AT 16:13:19 ON 07 JUN 2010 L51 10 S L45 STRUCTURE UPLOADED L52 S L52 FILE 'REGISTRY' ENTERED AT 16:16:10 ON 07 JUN 2010 FILE 'CAPLUS' ENTERED AT 16:16:10 ON 07 JUN 2010 L53 STRUCTURE UPLOADED S L53 FILE 'REGISTRY' ENTERED AT 16:17:35 ON 07 JUN 2010 L54 23 S L53 FILE 'CAPLUS' ENTERED AT 16:17:36 ON 07 JUN 2010 L55 48 S L54 FILE 'REGISTRY' ENTERED AT 16:17:41 ON 07 JUN 2010  $\Rightarrow$  s sub=141 sam 155 SUBSET AND SAMPLE ARE IGNORED FOR THIS SEARCH L56 23 L54

SAMPLE SUBSET SEARCH INITIATED 16:18:14 FILE 'REGISTRY'

52 TO ITERATE

SAMPLE SUBSET SCREEN SEARCH COMPLETED -

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[2-[(1E)-2-[4(dimethylamino)phenyl]ethenyl]-5-thiazolyl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]
MF C25 H21 N5 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-(4-butylphenyl)ethenyl]-2-thiazolyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C33 H28 N4 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Acetamide, N-[5-[bis(2-hydroxyethyl)amino]-2-[2-[3,4-dibutoxy-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]diazenyl]phenyl]
MF C36 H43 N7 O6 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[butyl[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C26 H25 N5 O3 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1N 1,3-Isobenzofurandione, 5,5'-[2,2,2-trifluoro-1(trifluoromethyl)ethylidene|bis-, polymer with 2,4-diaminophenol
dihydrochloride, 6-[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5[(1E)-2-[4-cynno-5-(dicynomethylene)-2,5-dihydro-2-methyl-2-[3-[[4[(trifluoroethenyl)oxy]benzoyl]oxy]propyl)-3-furanyl]ethenyl]-2thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylylamino]hexyl
1,2-benzenedicarboxylate (ester) 4-[(trifluoroethenyl)oxy]benzoate
(ester)

MF C73 HB1 F3 N4 O12 S2 . x (C19 H6 F6 O6 . C6 H8 N2 O . 2 C1 H)x . x C9 H5
F3 O3

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

Double bond geometry as shown.

PAGE 1-B

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1H-Pyrrole-1-propanoic acid, 2,5-dihydro-2,5-dioxo-,
2-[[4-[2-[3-[[[3,5-bis[(2,3,4,5,6-pentafluorophenyl)methoxy]benzoyl]oxy]methyl]-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylamino]ethyl ester

MF C57 H36 F13 N5 O9 S

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CM

CM

●2 HC1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

PAGE 3-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,4,5-tris[(2-ethylhexyl)oxy]-,
 [8-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-8-'-[[12]-2-[4-(dibtyllamino)phenyl]ethenyl][6,6'-bi-2H-thieno[3,4-b][1,4]dioxepin]-3,3'(4H,4'H)-diylidene]tetrakis(methylene)
 ester (9CI)

MF C170 H260 N4 025 S2

Double bond geometry as shown.

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C34 H33 F3 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 O5 S2

Double bond geometry as shown.

N(Bu-n)2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S S1

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2(acetyloxy)ethyl]amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl]-3cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C40 H46 N4 O5 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C42 H54 N4 O3 S2 S12

Double bond geometry as shown.

PAGE 1-B

PAGE 1-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[(1-oxo-2-propen-1-y1)oxy]-,
 [2-[2-[4-[[2-[[3,5-bis[(1-oxo-2-propen-1-y1)oxy]-benzoy1]oxy]ethyl]ethylamino]phenyl]ethenyl]-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-3-thienyl]methyl ester

MF C55 H41 F3 N4 013 S

PAGE 1-A
$$H_2C = CH - C - CH = CH_2$$

$$CH_2$$

$$CH_3$$

$$CH_4$$

$$CH_2$$

$$CH_3$$

$$CH_4$$

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued) \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[(1-oxo-2-propen-1-y1)oxy]-,
[5-[2-[4-[[2-[[3,5-bis[(1-oxo-2-propen-1-y1)oxy]+ny]-]+]-]-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-3-thienyl]methyl ester

MF C55 H41 F3 N4 013 S

PAGE 1-A

$$\begin{array}{c} \text{CN} & \text{Me} \\ \text{NC} & \text{CF}_3 \\ \text{NC} & \text{CH} \\ \text{CH} \\ \text{CH} & \text{CH}_2\text{-O-C} \\ \text{CH} \\ \text{CH} \\ \text{CH} \end{array}$$

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-[1-(phenylmethyl)-1H-pyrrol-2-yl]ethenyl]-2(5H)-furanylidene]
NF C23 H8 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[2-[5-[2-[1-(phenylmethyl)-1H-indol-3-y]]ethenyl]-2-thienyl]ethenyl]-2(5H)-furanylidene]-MF C33 H24 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[4-[2-[5-[2-[4-[bis(4-iodophenyl)amino]phenyl]ethenyl]2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C36 H24 I2 N4 O S
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2=[3-cyano-4-{(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[(6-[((1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidenel)

MF C60 H81 F3 N4 O6 S2 Si

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L57 23 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(3,4-dimethyl]phenyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C48 H50 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1): HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

L11

L12

```
=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
    FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
               STRUCTURE UPLOADED
L1
             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
L10
             0 S L3 AND L9
```

26 S ELECTRO-OPTIC CHROMOPHORES

12 S L4 OR L9

L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37 L38		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41 L42	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL 54 S L41 AND C5N/RF
L43	FILE	'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010 20 S L42

L56 23 S SUB=L41 SAM L55 L57 23 S SAM L53 SUB=L41

=> s sub=141 full 153

FULL SUBSET SEARCH INITIATED 16:19:23 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 947 TO ITERATE

100.0% PROCESSED 947 ITERATIONS 471 ANSWERS SEARCH TIME: 00.00.01

L58 471 SEA SUB=L41 SSS FUL L53

=> s 158 not 142

L59 424 L58 NOT L42

=> s 158 not 45 98757 45

L60 471 L58 NOT 45

=> d scan 1-

'1-' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-(1-piperidinyl)ethenyl]-2(5H)-furanylidene]MF C17 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

EPROP - Table of experimental properties PPROP - Table of predicted properties PROP - EPROP, ETAG, PPROP

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification

```
L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)
PATS -- PI, SO
STD -- BIB, IPC, and NCL
```

IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX Format is the same as ALL plus SPEC.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d scan

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN INDEX NAME NOT YET ASSIGNED
MF C111 H117 N9 03 S3

Double bond geometry as shown.

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

PAGE 1-A

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2000

L60 471 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
Propanedinitrile, 2=[3-cyano-4-[2-[5-[2-[5-[4-[2-[[(1,1-dimethylathylloxy]ethyl]ethylamino]phenyl]-2-thienyl]+thenyl]-3-[[(1,1-dimethylathyllothylathyllo

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2={3-cyano-5,5-dimethyl-4-[(1E)-2-(1-piperidinyl)-ethenyl)-2(5H)-furanylidene]-, hydrate (50:19)
MF C17 H18 N4 O . 19/50 H2 O

Double bond geometry as shown.

●19/50 H2O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis[3-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]propyl]amino]phenyl]ethenyl]-3,4-dibutoxy2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5-[4(methoxymethoxy)phenyl]-5-(trifluoromethyl)-2(5H)-furanylidene]MF C71 H97 F3 N4 O9 S2 S12

Double bond geometry as shown.

PAGE 1-A

$$\begin{array}{c} \text{N-BuO} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CH}_2)_3 \\ \text{(CH}_2)_3 \\ \text{N-BuO} \\$$

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-4-[5-[4-cyano-5-(dicyanomethyl)-2,2-dimethyl3(2H)-furanylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-,
ion(1-)
MF C25 H17 N6 O2
CT CCM

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[2-[(1E)-2-[5-[(1E)-2-(4-butylphenyl)ethenyl]-2-thienyl]ethenyl]-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C33 H28 N4 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzenesulfonic acid, 4-methyl-, compd. with
2-[3-cyano-5,5-dimethyl-4-[2-[5-(1-piperidinyl)-2-thienyl]ethenyl]-2(5H)furanylidene]propanedintrile, ion(1-) (1:1)
MF C21 H20 N4 O S . C7 H7 O3 S

CM 1

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CM

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[5-[2-[4-[bis(2-

mercaptoethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]-, polymer with
1,1'-(2,2',3,3',5,5',6,6'-octafluoro[1,1'-biphenyl]-4,4'-diyl)bis[1H-pyrrole-2,5-dione] and 4,4'-thiobis[benzenethiol]
MF (C47 H52 C12 N4 O S3 . C20 H4 F8 N2 O4 . C12 H10 S3)x
CI FMS

CM 1

PAGE 1-A

PAGE 2-A

PAGE 1-A

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]diazenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C26 H24 N6 O3 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Ferrocene, 1,1'-bis([1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-phenyl-2-(triflloromethyl)-3-furanyl]ethenyl]
MF C44 H22 F6 Fe N6 O2

C1 CS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-[[(1,1-dimethylethyl]dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C40 H54 N4 O3 S Si2

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\* <------User Break----->

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L60 471 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Furancarboxylic acid, 3,3'-[5-[[[2-[2-[4-[[2-[3,5-bbis[(3-furanylcarbonyl)oxy]behryl]ethylamino]behnyl]ethenyl]-5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-(trifluoromethyl)-3-furanyl]ethenyl]-2-thienyl]methoxy]carbonyl]-1,3-phenylene] ester
MF C63 H41 F3 N4 O17 S

PAGE 1-A

L11

L12

```
=> d his
     (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010)
    FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010
               STRUCTURE UPLOADED
L1
             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
L10
             0 S L3 AND L9
```

26 S ELECTRO-OPTIC CHROMOPHORES

12 S L4 OR L9

L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37 L38		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41 L42	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL 54 S L41 AND C5N/RF
L43	FILE	'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010 20 S L42

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L56 23 S SUB=L41 SAM L55
L57 23 S SAM L53 SUB=L41
L58 471 S FULL L53 SUB=L41
L59 424 S L58 NOT L42
L60 471 S L58 NOT 45
```

=> s 160 and ed <= 2004 78285588 ED <= 2004

(ED<=20049999)

L61 132 L60 AND ED<=2004

=> d scan 1-

'1-' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl.6-hydroxyhexyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]-

C32 H34 N4 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 30 names
SQIDE - IDE, plus sequence data
SQIDE - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

EPROP - Table of experimental properties PPROP - Table of predicted properties PROP - EPROP, ETAG, PPROP

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued) STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available. The MAX format is the same as ALL plus SPEC. The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d scan

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-(3-cyano-4-[2-[5-(dihexylamino)-3-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C28 H36 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2000

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Phenol, 4-ethenyl-, homopolymer, 6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[[4-[(trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylamino|hexyl 1,2-benzenedicarboxylate 4-[(trifluoroethenyl)oxy]benzoate (9CI)
MF C73 H81 F3 N4 O12 S2 . x C9 H5 F3 O3 . x (C8 H8 O)x

CM 1

Double bond geometry as shown.

PAGE 1-B

CM 2

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[(1,1-dimethylsity]lowy]ethyl]amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]
MF C55 H74 C12 N4 O3 S Si2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-(3-cyano-4-[(2x, 4x, 6x, 8b)-8-[3-(2-hydroxyethyl)-2(3H)-benzothiazolylidene]-2, 4, 6-octatrien-1-yl]-5, 5-dimethyl-2(5H)-furanylidene]
MF C27 H24 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-3-[1-(2,3-dihydroxypropy1)-4(1H)-pyridinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C21 H20 N4 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
Propanedinitrile, 2=[4-[(1E)-2-[5'-[[6-[(1E)-2-[4-[bis[2-[[(1,1-dinethylathyl]antho]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C63 H88 N4 O5 S2 S12

Double bond geometry as described by E or Z.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl dichloride, 1,4,5,6,7,7-hexachloro-, polymer with

[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]propanedinitrile and 2,3,5,6-tetrachloro-1,4-benzenedimethanol (9CI)

MF (C43 H46 C12 N4 O3 S . C9 H2 C18 O2 . C8 H6 C14 O2)x

CI FMS

CM 1

Double bond geometry as shown.

CM

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2 [3-cyano-4-[2-[5' -[2-[4-(diethylamino)phenyl]ethenyl]3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF C44 H52 N4 0 S2

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S Si

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedintrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 O5 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2(acetyloxy)ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5dimethyl-2(5H)-furanylidene]MF C32 H30 N4 O5 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(4-pyridinyl)ethenyl]-2(5H)-furanylidene| MF C17 H12 N4 O

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl[6-

(methoxymethoxy)hexyl]amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-(3-hydroxypropyl)-5-methyl-2(5H)-furanylidene]MF C38 H44 N4 O4 S

PAGE 1-A

PAGE 1-B

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

CM 2

CM 1

Double bond geometry as shown.

PAGE 1-A

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[(1,1-dinethylsily]]oxy]ethyl]amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(2,4-difluorophenyl)-5-methyl-2(5H)-fivanyl)denbel. furanylidene] -C55 H74 F2 N4 O3 S Si2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5'-[(1E)-2-[4-

(diethylamino)phenyl]ethenyl]-3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]5,5-dimethyl-2(5H)-furanylidene]MF C44 H52 N4 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E)-4-(1-methyl-2(1H)pyridinylidene)-2-buten-1-yl]-2(5H)-furanylidene]
MF C20 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-3-[1-(2-hydroxyethyl)-4(1H)-quinolinylidene]-1-propen-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C24 H20 N4 O2

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[7-[(1E)-2-[4-[bis(4-

Double bond geometry as shown.

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[4-[2-[5'-[[6-[2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylailyl]oxy]ethyl]maino]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylldene]methyl]-3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-63 H88 M4 O5 S2 Si2

PAGE 1-A Me- (CH2) 5 (CH<sub>2</sub>)<sub>5</sub>-Me

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,2-Benzenedicarboxylic acid, 1-[6-[4-[(1E)-2-[3,4-dibutoxy-5-[(1E]-2-[(1E)-2-[(1E)-2-[(1E]-2-[(1E)-2-[(1E]-2-[(1E]-2-[(1E)-2-[(1E]-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[4-[(1,2,2-trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]benzoyl]ester

MF C73 H81 F3 N4 012 S2

CI CCM

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2[3-cyano-5-(4-cyclohexylphenyl)-4-[2-[3,4-dihexyl-5-[2[4-[methyl.(2-oxiranylmethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5methyl-2(SH)-furanylidene]MF C51 H60 N4 O2 S

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[2-[5-[2-(4-aminophenyl)ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-MF C24 H18 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C40 H46 N4 O5 S

Aco-CH2-CH2 Aco-CH2-CH2-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]NF C62 H90 N4 07 S2 Si2

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-,
3-[4-cyano-5-(dicyanomethylene)-3-[2-[5-[4-[4-[ethyl[6-

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

(n-Bu) 2N-

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C34 H33 F3 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

hydroxyethyl)amino]phenyl]-1,3-butadien-1-yl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]-MF C51 H60 N4 O3 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E)-6-(1-methyl-2(1H)-pyridinylidene)-2,4-hexadien-1-yl]-2(5H)-furanylidene]-MF C22 H20 N4 O

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5'-[[6-[(1E)-2-[4-

(dibutylamino)phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF CC5 H68 W4 O3 S2

Double bond geometry as described by E or  $\ensuremath{\text{Z}}$  .

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(4-methoxyphenyl)amino]phenyl]ethenyllthieno(3,2-b]thien-2-yl]ethenyl]-3-cyanodihydro-5,5-dimethyl-2(3H)-furanylidene]
MF C40 H32 N4 O3 S2

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-3-[1-[2-(acetyloxy)ethyl]-4(1H)pyridinylidene]-1-propen-1-yl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C22 H20 N4 03

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

[[3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propy
1]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]thienyl]ethenyl]phenyl]ethylamino]hexyl] ester

MF C89 H92 F6 N4 O15 S2
CI CCM

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-(2-furanyl)ethenyl]-5,5-dimethyl2(5H)-furanylidene]
MF C16 H11 N3 02

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[(1E)-2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C27 H24 N4 O2 S

Double bond geometry as described by  ${\tt E}$  or  ${\tt Z}\,.$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-hydroxymethyl) amino]phenyl]ethenyl]-3-(hydroxymethyl)-2-thienyl]ethenyl]-5,5-dibutyl-3-cyano-2(5H)-furanylidene]
MF C35 H40 N4 O4 S

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 07 S2

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Benzoic acid, 3,5—bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-, 3-[4-cyano-5- (dicyanomethylene)-3-[2-[6-[4-[4-[thyl(6-hydroxyhexyl)amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-2,5-dihydro-2-methyl-2-furanyl]propyl ester C61 H54 F6 N4 08 S

PAGE 2-A - (CH<sub>2</sub>)<sub>6</sub>-OH

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C36 H42 N4 O3 S
CI CCM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C41 H49 F3 N4 O2 S Si

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E,8E)-8-(1-methyl-2(1H)-pyridinylidene)-2,4,6-octatrien-1-yl]-2(5H)-furanylidene)
MF C24 H22 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]-MF C51 H60 N4 O3 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S Si

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E,3E)-5-(1-methyl-4(1H)-pyridinylidene)-1,3-pentadien-1-yl]-2(5H)-furanylidene]
MF C21 H18 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[(4-[(1,2,2-trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]benyl]ethenyl]-2-thienyl]benyl]ethenyl]ethenyl] 2-(4-ethenylphenyl) ester MF C81 H87 F3 N4 O12 S2 CI CCM

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3-(hydroxymethyl)-2-thienyl]ethenyl]-5,5-dibutyl-3-cyano-2(5H)-furanylidene]
MF C35 H40 N4 O4 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2=[3-cyano-5,5-dimethyl-4-[(1E)-2-(2-thienyl)ethenyl]-2(5H)-furanylidene] - MF C16 H11 N3 O S

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-4-[[18]-2-[3,4-diethyl-5-[[18]-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene)MF C33 H36 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzoic acid, 3,5-bis(phenylmethoxy)-,

[[4-[2-[4-[[3,5-bis(phenylmethoxy)benzoyl]oxy]methyl]-5-[2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-2-thienyl]ethenyl]penyl]imino]di-2,1-ethanediyl ester (9CI)
MF CS8.888.W4.013 S

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Benzoic acid, 4-[(trifluoroethenyl)oxy]-,
[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9C1)

MF C68 H68 F6 N4 O11 S2

Double bond geometry as shown.

PAGE 1-A n-BuO OBu-n n-Bu0

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-oxiranylmethyl)amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C38 H42 N4 O3 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1,2-Benzenedicarboxylic acid,
1-[6-[4-[4-[5-[2-[2-[3-[13,5-biz[[4-[(1,2,2trifluoroethenyl) oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester

MF C69 H58 F6 N4 O11 S
CI CCM

PAGE 1-A CF2

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidenelMF C28 H26 N4 O S

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]MF C65 H92 N4 O3 S Si2

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Tricyclo[3.3.1.13,7]decane-1-carboxylic acid, [5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-3-thienyl]methyl ester C46 H52 N4 O3 S

PAGE 1-A N(Bu-n)2

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(2E,4E)-4-[1-(2,3-dihydroxypropyl)-2(1H)-pyridinylidene]-2-buten-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C22 H22 N4 03

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(1E,3E,5E)-7-(1-methyl-4(1H)pyridinylidene)-1,3,5-heptatrien-1-yl]-2(5H)-furanylidene]MF C23 H20 N4 O

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Benzoic acid, 3,5-bis(phenylmethoxy)-,

[[4-[(1E)-2-[4-[[[3,5-bis(phenylmethoxy)bozzoyl]oxy]methyl]-5-[(1E)-2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI)

MF C98 H88 N4 013 S

Double bond geometry as shown.

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PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,2-Benzenedicarboxylic acid, 6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[3,4-[(1E)-2-[2,4-[(1E)-2-[2,4-[(1E)-2-[2,4-[(1E)-2-[2,4-[2,4-[2,4-[2,4]-2-[2,4-[2,4]-2-[2,4-[2,4]-2-[2,4-[2,4]-2-[2,4-[2,4]-

dibutoxy-5-[(1E)-2-[4-equano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[4-[(trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethenyl]phenyl]ethenyl]phenyl]ethenyl]phenyl ester, polymer with 4-ethenylphenyl 4-[(trifluoroethenyl)oxy]benzoate (9CI)
MF (C81 H87 F3 N4 O12 S2 . C17 H11 F3 O3)x
CI PMS

$$\stackrel{\mathsf{CF2}}{\Vdash} \mathsf{C} = \mathsf{CH2}$$

CM 2

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-(3-thienyl)ethenyl]2(5H)-furanylidene]
MF C16 H11 N3 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Benzolc acid, 3,5-bis(phenylmethoxy)-, [[4-[2-[5-[2-[2-[4-[1]3,5-bis(phenylmethoxy)benzoyl]oxy]butyl]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3,4-dibutyl-2-thienyl]phenyl]imino]di-2,1-ethanediyl ester (9CI) C102 H96 N4 O13 S

PAGE 1-B

- Ph

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

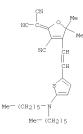
L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3, 4-dipropyl-2-thienyl]ethenyl]-5, 5-dimethyl-2(5H)-furanylidene]
MF C35 H40 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5-(dihexylamino)-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C28 H36 N4 O S



L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5-(4-hydroxybutyl)-5-methyl-2(5H)-furanylidene]-MF C51 H76 N4 O4 S Si2 COM

PAGE 1-B

 $\sim$  (CH<sub>2</sub>)<sub>4</sub>-OH

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C34 H36 N4 O2 S

PAGE 1-A

PAGE 1-B

— CN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E,3E)-4-[4-[bis[2-[[(1,1-

Double bond geometry as shown.

PAGE 1-A (CH<sub>2</sub>)5 (CH<sub>2</sub>)5

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[(2E,4E,6E)-6-[1-(2,3-dihydroxypropyl)-

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benroic acid, 3,5-bis[(2-ethylhexyl)oxy]-,
[5=[2-[4-eyano-5-(dicyanomethylen-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-3-thienyl]methyl ester

MF C58 H74 N4 OS S

PAGE 1-A

PAGE 2-A

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 3-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

No Propanedinitrile, 2-[3-cyano-4-[(1E,3E)-5-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
NF C23 H22 N4 O3

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-

(diethylamino)phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]-MF C30 H26 N4 O S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-C

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[3-

[[3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propy
1]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]ethenyl]ethylamino]hexyl] 2-(4-ethenylphenyl) ester
MF C97 H98 F6 N4 O15 S2
CI CCM

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5'-[[3-[2-[4-

(dimethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]methyl]3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF C51 H60 N4 O S2

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile,
2-[3-cyano-4-[(1E)-2-[3,4-dibutyl-5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidenelMF C37 H44 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Carbamic acid, (3-isocyanato-4-methylphenyl)-,
[[4-[2-[5-[2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-4-[[[[(3-isocyanato-4-

methylphenyl)amino]carbonyl]oxy]methyl]-2-thienyl]ethenyl]phenyl]imino]di2,1-ethanediyl ester (9CI)
MF C62 H58 N10 O10 S
CI CCM

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

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PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl(2-hydroxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C28 H26 N4 O2 S

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, [4-[2-[5-[2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-

thienyl]ethenyl]-3-cyano-5-(4-hydroxybutyl)-5-methyl-2(5H)-furanylidene]-, polymer with 2,4-diisocyanato-1-methylbenzene and 2,2',2''-nitriiotris[ethanol] (9CI)
MF (C51 H76 N4 O4 S Si2 . C9 H6 N2 O2 . C6 H15 N O3)x
CI PMS

CM 1

PAGE 1-A

PAGE 1-B

 $\sim$  (CH<sub>2</sub>)<sub>4</sub>-OH

CM 2

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl[6-

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2={4-[2-[5-[2-[4-[bis(2-hydroxyethyl) amino]phenyl]-3, 4-bis(2, 2, 3, 3, 4, 4, 4-heptafluorobutoxy)-2-thienyl]ethenyl]-3, 4-bis(2, 2, 3, 3, 4, 4, 4-heptafluorobutoxy)-2-thienyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5, 5-dimethyl-2(5H)-furanylidene]
MF C50 H48 F14 N4 O7 S2

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[(1E)-2-[3,4-dihexyl-

5-[(1E,3E)-4-[4-[(2-hydroxyethyl)methylamino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]MF C52 H62 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[(1E, 3E, 5E)-5-[1-(2-hydroxyethyl)-4(1H)-quinolinylidene]-1,3-pentadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]-MF C26 H22 N4 O2

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C42 H54 N4 O3 S2 S12

Double bond geometry as shown. PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-C

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1,2-Benzenedicarboxylic acid, 6-[[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[2-[3-[[3,5-bis [[4-[(trifluoroethenyl)oxy]pheny]]methoxy]benzoyl]oxy]propyl]-d-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]phenyl]ethylamino]hexyl 4-ethenylphenyl ester, polymer with 4-ethenylphenyl 4-[(trifluoroethenyl)oxy]benzoate (9CI)

MF (C97 H98 F6 N4 O15 S2 . C17 H11 F3 O3)x

CM 1

Double bond geometry as shown.

PAGE 1-A

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

CM

$$\begin{array}{c} \operatorname{CF}_2 \\ | \\ \operatorname{F-C-O} \\ \\ | \\ \operatorname{C-O} \\ \end{array}$$

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(2-thienyl)ethenyl]-2(5H)-

furanylidene] -C16 H11 N3 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[[6-[(1,1-dimethylatiy])oxy]hexyl]ethylamino]phenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-5-(3-hydroxypropyl)-5-methyl-2(5H)-furanylidenel)

MF C62 H88 N4 07 S2 Si

Double bond geometry as shown.

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Carbamic acid, (3-isocyanato-4-methylphenyl)-,
[[4-[2-[5-[2-[2-2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3furanyl]ethenyl]-4-[[[[(3-isocyanato-4-

methylphenyl)amino]carbonyl]oxy]methyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester, polymer with 2,4-diisocyanato-1-methylbenzene and 2,2',2''-nitrilotris[ethanol] (9CI)
MF (C62 H58 N10 O10 S . C9 H6 N2 O2 . C6 H15 N O3)x
CI PMS

PAGE 1-A

CM 1

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-A

CM 2

см з

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

$$\begin{array}{c} {\rm CH_2-CH_2-OH} \\ | \\ {\rm HO-CH_2-CH_2-N-CH_2-CH_2-OH} \end{array}$$

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene)MF C32 H34 N4 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-1)-2-[4-[bis(2-[bis(2-[bis(2-1)-2-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C36 H42 N4 O3 S
CI CCM

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[4-[5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester
MF C42 H40 N4 O5 S
CI CCM

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2-

thienyl]ethenyl]-3-cyano-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]-MF C40 H51 F3 N4 O3 S Si2

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N Propanedinitrile,
2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E)-6-(1-methyl-2(1H)-quinolinylidene)-2,4-hexadien-1-yl]-2(5H)-furanylidene]
MF C26 H22 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-(3-cyano-4-[(1E)-2-[3,4-dihexyl-5-[(1E)-2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5-methyl-5-(2,3,4,5,6-penthafluorophenyl)-2(5H)-furanylidene]
MF C44 H45 F5 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S

Double bond geometry as shown.

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile,
2-[3-cyano-4-[(1E,3E,5E,7E)-7-[1-(2-hydroxyethyl)-4(1H)quinolinylidene]-1,3,5-heptatrien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]MF C28 H24 N4 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile,
2 [3-cyano-5-(4-cyclohexylphenyl)-4-[(1E,3E)-4-[5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yll-5-methyl-2(5H)-furanylidene]MF C53 H64 N4 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene)MF C36 H42 N4 O3 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-(1H-indol-2-y1)ethenyl]-5,5-dimethyl2(5H)-furanylidene]
MF C20 H14 N4 O

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 4-[(1,2,2-trifluoroethenyl)oxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furanyl]propyl ester
MF C71 H91 F3 N4 O9 S2 Si

Double bond geometry as shown.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C34 H33 F3 N4 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[2-(1,3-benzodioxol-5-yl)ethenyl]-3-cyano-5,5dimethyl-2(5H)-furanylidene]
MF C19 H13 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C40 H46 N4 O5 S

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Phenol, 4-ethenyl-, homopolymer,
6-[[4-[4-[5-[2-[2-[3-[3-5-1x[[4-[(1-2,2trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-cyano-5-

CM 1

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

CM 4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-(2-furanyl)ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF C16 H11 N3 02

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-

dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]-MF C34 H30 N4 O3 S

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(2E,4E,6E,8E)-8-(1-methyl-2(1H)-quinolinylidene)-2,4,6-octatrien-1-yl]-2(5H)-furanylidene)MF C28 H24 N4 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2=[3-cyano-4-[(2E,4E)-4-[3-(2-hydroxyethyl)-2(3H)-benzothiazolylidene]-2-buten-1-yl]-5,5-dimethyl-2(5H)-£uranylidene]
MF C23 H20 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[2-[5-[[3-[2-[4-

(diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]methyl]-3,4-dihexyl-2-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]-MF C60 H74 N4 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-MF C36 H42 N4 O5 S

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile,
2-[3-cyano-5-(3,4-dichlorophenyl)-4-[(1E,3E)-4-[5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,4-dihexyl-2-thienyl]-1,3-butadien-1-yll-5-methyl-2[(5B)-furanylidene]
MF C47 H52 C12 N4 O S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2={4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl) amino] phenyl] ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]
C43 B46 C12 N4 O3 S
CFI COM

Double bond geometry as shown

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furanyl]propyl ester
MF C87 H102 F6 N4 O12 S2 Si

Double bond geometry as shown.

PAGE 1-A

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued) PAGE 2-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-(3-furanyl)ethenyl]-5,5-dimethyl-2(5H)furanylidene]MF C16 H11 N3 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Si\_Bu-t

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)]pheny]-1,3-butadien-1-yl]-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5
MF C41 H49 F3 N4 O2 S Si

N(Bu-n)2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C32 H30 N4 O5 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Phenol, 4-ethenyl-, homopolymer, benzoate
6-[4-[4-[5-[2-[4-cyano-5-cdicyanomethylene)-2,5-dihydro-2,2-dimethyl-3furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl
1,2-benzenedicarboxylate
MF C42 H40 N4 O5 S . x (C8 H8 O)x . x C7 H6 O2

CM 1

PAGE 1-B

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-(3-cyano-5,5-dimethyl-4-[2-(2-pyridinyl)ethenyl]-2(5H)-furanylidene) MF C17 H12 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid,
4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(1,3-dihydro-1,3-dioxo-2R-isoindole-5,2-diyl)]bis-, polymer with
[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-diyl)]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]propanedinitrile (9CI)

MF (C34 H30 N4 O3 S . C33 H16 F6 N2 O8)x

CI PMS

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

CM 2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[2-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]diazenyl]-4-chloro-5-thiazolyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-MF C25 H22 C1 N7 03 S

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedimitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[2-[5-[3-[3-[2-[4-(diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-propen-1-yl]-3,4-dihexyl-2-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]-MF C62 H76 N4 O S

NC CH (CH2)5-Me

PAGE 1-A

PAGE 2-A

Et 2N Me

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, [3-cyano-4-[(1E)-2-[[[[1,1dimethylethyl)dimethylsilyl]oxy]methyl]-7-[(1E)-2-[4-[ethyl(2hydroxyethyl)amino]phenyl]ethenyl]-2,3-dihydrothieno[3,4-b]-1,4-dioxin-5yl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (9CI)

CI 1DS

CI 1DS

PAGE 1-A

PAGE 1-A

PAGE 1-A

CH

CH

CH

CH

CH

CH

CN

PAGE 2-A
O-CH<sub>2</sub>-D1
Me-Si-Bu-t
Me

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(2E,4E,6E)-6-[3-(2-hydroxyethyl)-2(3H)-benzothiazolylidene]-2,4-hexadien-1-yl]-5,5-dimethyl-2(5H)-furanylidene]
MF C25 H22 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-3-(1-methyl-4(1H)-pyridinylidene)-1-propen-1-yl]-2(5H)-furanylidene]
MF C19 H16 N4 O

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]-MF C41 H42 C12 N4 O3 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(3-thienyl)ethenyl]-2(5H)furanylidene] 
MF C16 H11 N3 O S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 4-[(1,2,2-trifluoroethenyl)oxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2thienyl]ethenyl]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2furanyl]propyl ester

MF C65 H77 F3 N4 09 S2

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C34 H36 N4 O S

Double bond geometry as shown.

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, [4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-, polymer with 1,3-diisocyanatomethylbenzene (9CI) MF (C36 H42 N4 O3 S . C9 H6 N2 O2)x

\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*

CM 1

Double bond geometry as shown.

CM 2

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[2-(3-pyridinyl)ethenyl]-2(5H)-furamylidene] MF C17 H12 N4 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

L61 132 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[4-[2-[5-[2-[4-[[3-[2,5-bis[[(1,1-

dimethylethyl)dimethylsilyl]oxy]phenyl]propyl]methylamino]phenyl]ethenyl]2-thlenyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]MF C46 H58 N4 O3 S Si2

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10

L11

L12

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             0 S L1
L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
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26 S ELECTRO-OPTIC CHROMOPHORES

0 S L3 AND L9

12 S L4 OR L9

L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37 L38		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41 L42	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL 54 S L41 AND C5N/RF
L43	FILE	'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010 20 S L42

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L56
            23 S SUB=L41 SAM L55
L57
            23 S SAM L53 SUB=L41
L58
            471 S FULL L53 SUB=L41
           424 S L58 NOT L42
L59
            471 S L58 NOT 45
L60
L61
            132 S L60 AND ED<=2004
=> s 161 not 145
          131 L61 NOT L45
L62
=> s 161 not 142
           118 L61 NOT L42
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=> file caplus FILE 'CAPLUS' ENTERED AT 16:23:30 ON 07 JUN 2010 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

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```
164 116 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN

CC 75-8 (Crystallography and Liquid Crystals)
Section cross-reference(s): 22, 27, 73

1 A non-linear optical chromophore. 2-[3-cyano-4-((E)-(5-[4-(diethylamino)styry]|thiophen-2-y]|vinyl)-5,5-dimethylfuran-2-(5H)-ylidene]propanedinitrile

ST mol structure cyanodiethylaminostyrylthiophenylvinyl methylfuranylidene propanedinitrile nonlinear optical material; crystal structure cyanodiethylaminostyrylthiophenylvinyl methylfuranylidenepropanedinitrile

TN Nonlinear optical material; crystal structure
(crystal structure
(cf[cyano([(diethylamino)styryl]thiophenyl]vinyl)dimethylfuranylidenepropanedinitrile)

TC Crystal structure
(lofe crystal structure
(lofe crystal structure)
(cf[cdiethylamino)styryl]thiophenyl)vinyl)dimethylfuranylidene
(crystal and mino structure of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN7 (1):1
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L64 116 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
high-β nonlinear optical chromophore-polymer guest-host materials
and dye spacer length effects in an amorphous polycarbonate copolymer
host)

IT 473796-78-0, LMCO 4H6m 676256-53-4, LMCO 4B6m
676256-54-5, LMCO 4H6m 676256-55-6, LMCO 4H6m
RL: PRP (Properties); TEM (Technical or engineered material use); USES
(Uses)
(dopant; near-IR optical-absorption behavior in high-β nonlinear
optical chromophore-polymer guest-host materials and dye spacer length
effects in an amorphous polycarbonate copolymer host)

IT 132721-26-7, Bisphenol A-carbonic
acid-3-3,5-trimethylcyclohexanebisphenol
copolymer
RL: PRP (Properties); TEM (Technical or engineered material use); USES
(Uses)
(polymer host; near-IR optical-absorption behavior in high-β
nonlinear optical chromophore-polymer guest-host materials and dye
spacer length effects in an amorphous polycarbonate copolymer host)

```
164 116 ANSWERS CAPLUS COPYRIGHT 2010 ACS on STN
CC 73-4 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 36
TI Near-infrared optical-absorption behavior in high-beta nonlinear optical chromophore-polymer guest-host materials. II. Dye spacer length effects in an amorphous polycarbonate copolymer host
ST near IR nonlinear optical dye homologous series polycarbonate host
Electrooptical absorption

(IR; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Dipole moment

(difference between ground and excited state; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Free energy

(excess, and inhomogeneous peak width; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Folycarbonates, properties
Ri-PRP (Properties)
(host; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Molecular structure-property relationship

(inhomogeneous width vs. dye alkyl spacer length; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Thermodynamic activity
(interaction coefficient vs. loss-concentration slope; near-IR optical-absorption behavior in high-β nonlinear optical chromophore-polymer guest-host materials and dye spacer length effects in an amorphous polycarbonate copolymer host)
IT Qualine dyes<
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Henry's law
(vs. loss-concentration slope; near-IR optical-absorption behavior in

L10

L11

L12

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L2
L3
            14 S L1 FULL
    FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010
L4
            11 S L3
    FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010
    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN : 172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
          172 SEA L5
L6
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
L8
             0 S OTOPHORE
L9
             1 S OPTOPHORE
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26 S ELECTRO-OPTIC CHROMOPHORES

0 S L3 AND L9

12 S L4 OR L9

L29 L30	FILE	'CAPLUS' ENTERED AT 15:18:50 ON 07 JUN 2010 90 S L27 13 S L28
L31	FILE	'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010 1 S L27 AND HYDROXYETHYL
L32 L33 L34 L35 L36 L37 L38		'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010 6 S L31 19 S L32 OR L30 4286 S MEROCYANINE 91 S L34 AND REVIEW/DT 0 S L35 AND FURNA 0 S L35 AND FURAN 9 S L34 AND FURAN
	FILE	'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
L39 L40 L41 L42	FILE	'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010 STRUCTURE UPLOADED 50 S L39 947 S L39 FULL 54 S L41 AND C5N/RF
L43	FILE	'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010 20 S L42

provided by InfoChem.

L56

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L57
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L58
           471 S FULL L53 SUB=L41
           424 S L58 NOT L42
L59
           471 S L58 NOT 45
L60
           132 S L60 AND ED<=2004
L61
            131 S L61 NOT L45
L62
L63
            118 S L61 NOT L42
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L64
           116 S L63
=> s 164 and pd<=2003
      23988064 PD<=2003
                (PD<=20039999)
            53 L64 AND PD<=2003
L65
=> file reg
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23 S SUB=L41 SAM L55

STRUCTURE FILE UPDATES: 3 JUN 2010 HIGHEST RN 1226953-63-4

Property values tagged with IC are from the ZIC/VINITI data file

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    FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010
L5
               TRA L4 1- RN :
                                  172 TERMS
    FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010
L6
           172 SEA L5
L7
             1 S L3 NOT L6
    FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010
             0 S OTOPHORE
L8
             1 S OPTOPHORE
L9
L10
             0 S L3 AND L9
L11
            12 S L4 OR L9
L12
            26 S ELECTRO-OPTIC CHROMOPHORES
L13
             0 S ELECTROPTIC CHROMOPHORES
L14
            27 S ELECTROOPTIC CHROMOPHORES
L15
         11072 S ELECTROOPTIC
L16
           660 S L15 AND CHROMOPHORE
L17
           679 S L12 OR L14 OR L16
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L18
        269403 S C6N/RF
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L32
            6 S L31
            19 S L32 OR L30
L33
L34
          4286 S MEROCYANINE
L35
            91 S L34 AND REVIEW/DT
L36
             0 S L35 AND FURNA
             0 S L35 AND FURAN
L37
L38
             9 S L34 AND FURAN
    FILE 'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
    FILE 'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010
L39
               STRUCTURE UPLOADED
L40
            50 S L39
           947 S L39 FULL
L41
            54 S L41 AND C5N/RF
L42
    FILE 'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010
L43
            20 S L42
    FILE 'REGISTRY' ENTERED AT 16:12:09 ON 07 JUN 2010
L44
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L45
             19 S L41 AND C3NS/RF
L46
              0 S L41 AND C3NSE/RF
             0 S L41 AND C3SEN/RF
L47
L48
             0 S L41 AND SE/ELS
L49
             0 S L41 AND SE/ES
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FILE 'CAPLUS' ENTERED AT 16:23:30 ON 07 JUN 2010 L64 116 S L63

L65 53 S L64 AND PD<=2003

FILE 'REGISTRY' ENTERED AT 16:24:06 ON 07 JUN 2010

FILE 'CAPLUS' ENTERED AT 16:24:12 ON 07 JUN 2010 L66 TRA L65 1- RN : 627 TERMS

FILE 'REGISTRY' ENTERED AT 16:24:25 ON 07 JUN 2010 627 SEA L66

=> s 167 and 164

L68 95 L67 AND L64

=> d scan

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2=[4-[2-[5-[2-[4-[bls(2-hydroxyethyl)amino]phenyl]+ethenyl]-3,4-bie(2,2,3,3,4,4,4-heptafluorobutoxy)-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H48 F14 N4 O7 S2

PAGE 1-B

PAGE 1-B

~ N- CH<sub>2</sub>- CH<sub>2</sub>- ОН | | СН<sub>2</sub>- СН<sub>2</sub>- ОН

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

CM 2

ом з см 4 L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Phenol, 4-ethenyl-, homopolymer,
6-[[4-{(12)-2-[5-(12)-2-[5-(12)-2-[2-[3-(12)-2-[3

CM 1

Double bond geometry as shown.

PAGE 1-A

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

1, 2-Benzenedicarboxylic acid, 6-[[4-[(1E]-2-[5-[(1E)-2-[5-[(1E)-2-[2-[3-[[3,5-bis[[4-[(trifluoroethenyl)oxy]phenyl]methoxylbenzoyl]oxy]propyl]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-4-[vibranyl]henyl]ethenyl) ester, polymer with 4-ethenylphenyl 4-[(trifluoroethenyl)oxy]benzoate (9CI)

MF (C97 H98 F6 N4 O15 S2 . C17 H11 F3 O3)x

CM 1

Double bond geometry as shown.

PAGE 1-A

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 1-C

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

CM

$$\begin{array}{c} \operatorname{CF}_2 \\ \\ \\ \operatorname{F-C-O} \\ \\ \end{array}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

[[3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propy
1]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-benyl]ethylamino]hexyl] ester

CB B92 F6 N4 O15 S2
CI CCM

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued) PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroetheny1)oxy]pheny1]methoxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furanyl]propyl ester
MF C87 H102 F6 N4 O12 S2 Si

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[[6-[(1,1-dimethylatily]loxy]hexyl]ethylamino]phenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-5-(3-hydroxypropyl)-5-methyl-2(5H)-furanylidenel)

MF C62 H88 N4 O7 S2 Si

Double bond geometry as shown.

PAGE 1-B

PAGE 1-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3,4-dipropyl-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]C35 H40 N4 O2 S

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[(1E)-2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C27 H24 N4 O2 S

Double bond geometry as described by E or  ${\mbox{\bf Z}}\,.$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)]phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dinethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C41 H52 N4 O2 S S1

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)]pheny]]-1,3-butadien-1-yl]-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]
MF C41 H49 F3 N4 O2 S Si

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

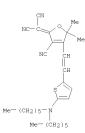
L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethy1(6-hydroxyhexy] amino]phenyl]ethenyl]]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C32.843 M4 O2 S

-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Propanedinitrile, 2-[3-cyano-4-[2-[5-(dihexylamino)-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]-MF C28 H36 N4 O S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 07 S2

Double bond geometry as shown.

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PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Phenol, 4-ethenyl-, homopolymer, benzoate
6-[[4-[4-[5-[2-[4-cyano-5-cdicyanomethylene)-2,5-dihydro-2,2-dimethyl-3furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl
1,2-benzenedicarboxylate
MF C42 H40 N4 O5 S . x (C8 H8 O)x . x C7 H6 O2

CM 1

PAGE 1-A (CH<sub>2</sub>)<sub>6</sub>—

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]
MF C50 H62 N4 O5 S2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN (Continued) HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[4-[5-[2-[4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester

MF C42 H40 N4 O5 S
C COM

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-, 3-[4-cyano-5-(dicyanomethylene)-3-[2-[5-[4-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-2,5-dihydro-2-methyl-2-furanyl]propyl ester C61 H54 F6 N4 08 S

PAGE 1-A

PAGE 2-A

- (CH<sub>2</sub>)<sub>6</sub>-OH

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]MF C34 H36 N4 O2 S

PAGE 1-A

PAGE 1-B

— CN

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

(Continued)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L68 95 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl[6-

PAGE 1-A

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

L28

=> d his (FILE 'HOME' ENTERED AT 14:57:21 ON 07 JUN 2010) FILE 'REGISTRY' ENTERED AT 14:57:36 ON 07 JUN 2010 L1 STRUCTURE UPLOADED L2 0 S L1 L3 14 S L1 FULL FILE 'CAPLUS' ENTERED AT 14:59:17 ON 07 JUN 2010 L411 S L3 FILE 'REGISTRY' ENTERED AT 14:59:29 ON 07 JUN 2010 FILE 'CAPLUS' ENTERED AT 14:59:33 ON 07 JUN 2010 L5TRA L4 1- RN : 172 TERMS FILE 'REGISTRY' ENTERED AT 14:59:34 ON 07 JUN 2010 172 SEA L5 L6 L7 1 S L3 NOT L6 FILE 'CAPLUS' ENTERED AT 15:00:42 ON 07 JUN 2010 L8 0 S OTOPHORE L9 1 S OPTOPHORE L10 0 S L3 AND L9 L11 12 S L4 OR L9 L12 26 S ELECTRO-OPTIC CHROMOPHORES L13 0 S ELECTROPTIC CHROMOPHORES L1427 S ELECTROOPTIC CHROMOPHORES L15 11072 S ELECTROOPTIC L16 660 S L15 AND CHROMOPHORE 679 S L12 OR L14 OR L16 L17 FILE 'REGISTRY' ENTERED AT 15:04:07 ON 07 JUN 2010 L18 269403 S C6N/RF FILE 'CAPLUS' ENTERED AT 15:04:59 ON 07 JUN 2010 TRA L17 1- RN : L19 3023 TERMS FILE 'REGISTRY' ENTERED AT 15:05:14 ON 07 JUN 2010 3023 SEA L19 L20 214 S L20 AND C5N/RF L21 L22 21 S L21 AND PROPANEDINITRILE 5 S L21 AND DICYANOMETHYLENE L23 25 S L22 OR L23 L24 L25 25 S L24 NOT L3 FILE 'CAPLUS' ENTERED AT 15:14:48 ON 07 JUN 2010 99 S L25 L26 FILE 'CAPLUS' ENTERED AT 15:15:01 ON 07 JUN 2010 FILE 'REGISTRY' ENTERED AT 15:16:51 ON 07 JUN 2010 L27 6 S L25 AND 5<=REF.CAPLUS

19 S L25 NOT L27

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L29
             90 S L27
L30
             13 S L28
    FILE 'REGISTRY' ENTERED AT 15:19:23 ON 07 JUN 2010
L31
             1 S L27 AND HYDROXYETHYL
    FILE 'CAPLUS' ENTERED AT 15:20:35 ON 07 JUN 2010
L32
             6 S L31
             19 S L32 OR L30
L33
           4286 S MEROCYANINE
L34
L35
             91 S L34 AND REVIEW/DT
L36
              0 S L35 AND FURNA
L37
              0 S L35 AND FURAN
L38
              9 S L34 AND FURAN
    FILE 'STNGUIDE' ENTERED AT 15:43:31 ON 07 JUN 2010
    FILE 'REGISTRY' ENTERED AT 16:06:27 ON 07 JUN 2010
L39
               STRUCTURE UPLOADED
L40
             50 S L39
           947 S L39 FULL
L41
            54 S L41 AND C5N/RF
L42
     FILE 'CAPLUS' ENTERED AT 16:09:52 ON 07 JUN 2010
L43
             20 S L42
    FILE 'REGISTRY' ENTERED AT 16:12:09 ON 07 JUN 2010
              0 S L41 AND C2NS/RF
L45
             19 S L41 AND C3NS/RF
              0 S L41 AND C3NSE/RF
L46
              0 S L41 AND C3SEN/RF
L47
L48
              0 S L41 AND SE/ELS
L49
              0 S L41 AND SE/ES
L50
              0 S L41 AND C2NO/RF
    FILE 'CAPLUS' ENTERED AT 16:13:19 ON 07 JUN 2010
L51
             10 S L45
               STRUCTURE UPLOADED
L52
                S L52
     FILE 'REGISTRY' ENTERED AT 16:16:10 ON 07 JUN 2010
     FILE 'CAPLUS' ENTERED AT 16:16:10 ON 07 JUN 2010
L53
                STRUCTURE UPLOADED
                S L53
     FILE 'REGISTRY' ENTERED AT 16:17:35 ON 07 JUN 2010
L54
             23 S L53
    FILE 'CAPLUS' ENTERED AT 16:17:36 ON 07 JUN 2010
L55
            48 S L54
     FILE 'REGISTRY' ENTERED AT 16:17:41 ON 07 JUN 2010
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23 S SUB=L41 SAM L55
L56
L57
            23 S SAM L53 SUB=L41
L58
           471 S FULL L53 SUB=L41
           424 S L58 NOT L42
L59
           471 S L58 NOT 45
L60
L61
           132 S L60 AND ED<=2004
           131 S L61 NOT L45
L62
L63
           118 S L61 NOT L42
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            116 S L63
L64
             53 S L64 AND PD<=2003
L65
     FILE 'REGISTRY' ENTERED AT 16:24:06 ON 07 JUN 2010
     FILE 'CAPLUS' ENTERED AT 16:24:12 ON 07 JUN 2010
L66
                TRA L65 1- RN :
                                    627 TERMS
     FILE 'REGISTRY' ENTERED AT 16:24:25 ON 07 JUN 2010
L67
           627 SEA L66
L68
            95 S L67 AND L64
=> file caplus
FILE 'CAPLUS' ENTERED AT 16:26:07 ON 07 JUN 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 7 Jun 2010 VOL 152 ISS 24
FILE LAST UPDATED: 6 Jun 2010 (20100606/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 165 cbib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 53 ANSWERS - CONTINUE? Y/(N):y

Double bond geometry as shown.

540777-78-4 CAPLUS

540777-78-4 CAPLUS Benzoic acid, 4-[(trifluoroethenyl)oxy]-, [[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]mino]di-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

540777-77-3 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyety])amin0]pheny1]=theny1]-3,4-dibutoxy-2-thieny1]etheny1]-3,4-dibutoxy-2-thieny1]etheny1]-3-cyano-5,5-dimethy1-2(5H)-furanylidene]-

INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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540777-76-2P 540777-77-3F IT

540777-76-2P 540777-77-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (fluorinated pi-bridge nonlinear optical chromophores and compns. and electrooptical devices using them) 540777-76-2 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

765317-91-7P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(fluorinated pi-bridge nonlinear optical chromophores and compns. and electrooptical devices using them)
76531-91-7 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3, 4-bis(2,2,3,3,4,4,4-heptafluorobutoxy)-2-thienyl]ethenyl]-3, 4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

PAGE 1-B

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2004:550794 Document No. 141:106890 Polymers having pendant nonlinear optical chromophores and electro-optic devices made from them. Huang, Diyun; Chen, Baoquan (Lumera Corporation, USA). U.S. Pat. Appl. Publ. US 20040132960 Al 20040708, 23 pp., Cont.-in-part of U.S. Pat. Appl. Publ. US (English). CODEN: USXXCO. APPLICATION: US 2003-625371 20030723. PRIORITY: US 2003-395610 20030324; US 2002-301978 20021122; US 20010813, US 2003 2003 2004

PRIORITY: 08 2003-39910 2003034, US 2002-301976 20021122; US -932831
20010817; US 2000-226267P 20000817.
The invention relates to a nonlinear optical chromophore having the formula D-π-A, wherein π is a π bridge including a thiophene ring having oxygen atoms bonded directly to the 3 and 4 positions of the thiophene ring, D is a donor, and λ is an acceptor, and compns. that include a linear polymer and the chromophore as a pendant group.
540777-74-0P
RL: INF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (chromophores; polymers having pendant nonlinear optical chromophores and electro-optic devices made from them)
540777-74-0 CAPLUS
Propamedintrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene] (CA INDEX NAME)

Double bond geometry as shown.

718637-00-4P IT 718636-99-8P

718636-99-8P 718637-00-4P RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (polymers having pendant nonlinear optical chromophores and electro-optic devices made from them) 718636-99-8 CAPLUS Phenol, 4-ethenyl-, homopolymer, 6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[[4-(trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl[ethenyl]ethenyl[ 1,2-benzene

CM 1

CRN 701235-61-2 CMF C73 H81 F3 N4 O12 S2

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

PAGE 1-B

CM 2

CRN 134151-66-9 CMF C9 H5 F3 O3

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 3

CRN 24979-70-2 CMF (C8 H8 O)x CCI PMS

CM 4

718637-00-4 CAPLUS

RN 718637-00-4 CAPLUS
CN Phenol, 4-ethenyl-, homopolymer,
6-[[4-[(1E)-2-[5-[(1E)-2-[5-((1E)-2-[2-[3[[3,5-bis[[4-[(trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3,4dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]phenyl]ethylamino|hexyl 1,2-benzenedicarboxylate
4-[(trifluoroethenyl)oxy]benzoate (9CI) (CA INDEX NAME)

CM 1

Double bond geometry as shown.

CRN 701235-63-4 CMF C89 H92 F6 N4 O15 S2

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L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CRN 134151-66-9 CMF C9 H5 F3 O3

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 24979-70-2 CMF (C8 H8 O)x CCI PMS

CM 4

CRN 2628-17-3 CMF C8 H8 O

540777-76-2P 540777-77-3P 540777-78-4P 701235-51-0P 701235-53-2P 701235-55-4P 701235-61-2P 701235-63-4P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);

(Reactant or reagent)
(polymers having pendant nonlinear optical chromophores and electro-optic devices made from them)
540777-76-2 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

540777-78-4 CAPLUS
Benzoic acid, 4-[(trifluoroethenyl)oxy]-,
[[4-[(IE)-2-[3,4-dibutoxy-5-[(IE)-2-[3,4-dibutoxy-5-[(IE)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]phenyl]phenyl]phenyl]mino]di-2,1-ethanediyl ester
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B

701235-51-0 CAPLUS Propanedinitrile, 2=[3-eyano-4-[(1E)-2-[3,4-dibutoxy-5-[1E]-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[2,4-dibutox

Double bond geometry as shown.

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

540777-77-3 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyety])amino]phenyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-

Double bond geometry as shown.

PAGE 1-B

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A n-BuO OBu-n (CH<sub>2</sub>)3 n-BuO

PAGE 1-B

701235-53-2 CAPLUS
Benzoic acid, 4-[(1,2,2-trifluoroethenyl)oxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thieny1]etheny1]-2-thieny1]etheny1]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furany1]propyl ester (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

701235-55-4 CAPLUS
Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

[[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl

]-2-thieny1]etheny1]-2-thieny1]etheny1]-5-(dicyanomethylene)-2,5-dihydro-2-methy1-2-furany1]propy1 ester (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

701235-59-8 CAPLUS Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroetheny1)oxy]pheny1]methoxy]-, 3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[ethy1(6-hydroxyhexy1)amino]pheny1]etheny1]-2-thieny1]etheny1]-2-thieny1]etheny1]-2-thieny1]popy1 ester (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-B

701235-57-6 CAPLUS Benzoic acid,  $4-[(1,2,2-\text{trifluoroethenyl}) \, \text{oxy}]$ -, 3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-thienyl]-2-thienyl]-2-thienyl]-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-2-thienyl]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thienyl]-3-(CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

701235-61-2 CAPLUS

1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[[4-[(1,2,2-trifluoroethenyl)oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]ethenyl] ester (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B

RN 701235-63-4 CAPLUS CN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[3-

 $\label{local-prop} \begin{tabular}{l} [ \{3,5-bis[\{4-[(1,2,2-trifluoroetheny1)oxy]pheny1]methoxy]benzoy1]oxy]propy \\ 1]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furany1]etheny1]-1. \\ \begin{tabular}{l} [ \{3,5-bis[\{4-[(1,2,2-trifluoroetheny1)oxy]pheny1]methoxy]benzoy1]oxy]propy \\ 1]-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furany1]etheny1]-1. \\ \end{tabular}$ 

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continues 3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]ethylamino]hexyl] ester (CA INDEX NAME) (Continued)

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

2004:471043 Document No. 141:44659 Second order nonlinear optical chromophores, polymers, and electro-optic devices. Huang, Diyun; Chen, Baoquan (Lumera Corporation, USA). PCT Int. Appl. NO 2004048927 A2

20040610, 36 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CM, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EG, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LK, LS, LT, LU, LV, MA, ND, MG, MK, MN, MM, MM, MX, MZ, NI, NO, NZ, CM, PG, FH, FL, FT, RO, RU, SC, SD, SE, SG, SK, SI, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RM: AT, BE, BF, BJ, CF, GG, GR, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, FT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.

APPLICATION: WO 2003-US37180 20031119. FRIORITY: US 2002-2002/301978 20021122; US 2003-2003/625371 20030723.

AB The invention refers to a nonlinear optical chromophore D-m-A, wherein m is a m bridge including a thiophene ring having 0 atoms bonded directly to the 3 and 4 positions of the thiophene ring, D is a donor, and

and

A is an acceptor, and compns. that include a linear polymer and the chromophore as a pendant group.
540777-78-49 701235-67-8P 701235-70-3P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (USES)
(second order nonlinear optical chromophores, polymers containing

same, and

, and
electro-optic devices therefrom)
540777-78-4 CAPLUS
Benzoic acid, 4-[(trifluoroethenyl)oxy]-,
[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]-2-thlenyl]ethenyl]ethenyl]ethenyl]phenyl]phenyl]mino]di-2,1-ethanediyl ester
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

$$\bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcap_{CF_2}^F$$

701235-67-8 CAPLUS 1,2-Benzenedicarboxylic acid, 6-[[4-[(1E)-2-[3,4-dibutoxy-5-[4]-2-[3,4-dibutoxy-5-[4]-2-[3,4-dibutoxy-5-[4]-2-[3,4-dibutoxy-5-[4]-2-[3,4-dibutoxy-5-[4]-2-[

dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[[4-([triflucroethenyl])oxy]benzoyl]oxy]propyl]-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]phenyl]ethylamino]hexyl 4-ethenylphenyl ester, polymer with 4-ethenylphenyl 4-[(triflucroethenyl)oxy]benzoate (9CI) (CA INDEX NAME)

CM 1

CRN 701235-66-7 CMF C17 H11 F3 O3

$$\begin{array}{c} \operatorname{CF}_2 \\ | \\ \operatorname{F-C-O} \end{array}$$
 
$$\operatorname{CH-CH}_2$$

CM 2

CRN 701235-65-6 CMF C81 H87 F3 N4 O12 S2

Double bond geometry as shown.

n-BuO

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) PAGE 1-A

PAGE 1-B

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

701235-70-3 CAPLUS 1,2=Benzenedicarboxylic acid, 6-[[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[3-[3.5-bls[[4-[(trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-eyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3,4-dibutoxy-2-thienyl]bethenyl]-3,4-dibutoxy-2-thienyl]phenyl]ethenyl]benylethylamino]hexyl 4-ethenylphenyl ester, polymer with 4-ethenylphenyl 4-[(trifluoroethenyl)oxy]benzoate (9CI) (CA INDEX NAME)

CM 1

CRN 701235-69-0 CMF C97 H98 F6 N4 O15 S2

Double bond geometry as shown.

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-C

PAGE 2-B

CM 2

CRN 701235-66-7 CMF C17 H11 F3 O3

$$\begin{array}{c} \operatorname{CF}_2 \\ \mathbb{H} \\ \operatorname{C-O} \end{array}$$

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

540777-76-2 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

701235-51-0 CAPLUS Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[6-[(1,1-dimethylethyl)dimethylsily]oxy]hexyl]ethylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B

701235-53-2 CAPLUS

Benzoic acid, 4-[(1,2,2-trifluoroethenyl)oxy]-, 3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thieny1]etheny1]-2-thieny1]etheny1]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furany1]propyl ester (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

540777-77-3 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyety])amino]phenyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

$$\begin{array}{c} \text{N-BuO} \\ \text{Me} \\ \text{Me} \\ \text{L-Bu} \end{array} \begin{array}{c} \text{Me} \\ \text{Me} \\ \text{E} \\ \text{E} \\ \text{S} \end{array} \begin{array}{c} \text{E} \\ \text{S} \\ \text{N-BuO} \end{array}$$

PAGE 1-B

701235-55-4 CAPLUS
Benzoic acid, 3/5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-,
3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-

 $\hbox{\tt [[6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]ethylamino]phenyl]ethenyl}$ 

]-2-thieny1]etheny1]-2-thieny1]etheny1]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-furany1]propyl ester (CA INDEX NAME)

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued) PAGE 2-B

701235-57-6 CAPLUS Benzoic acid,  $4-[(1,2,2-\text{trifluoroetheny1}) \, \text{oxy}]$ -,  $3-[4-\text{cyano}-3-[(1E)-2-[3,4-\text{dibutoxy}-5-[(1E)-2-[3,4-\text{dibutoxy}-5-[(1E)-2-[4-\text{theny1}]-6-\text{hydroxyhexy1}) \, \text{amino}] \, \text{pheny1}] \, \text{etheny1}]$ -2-thieny1]-12-thieny1]-2-thieny1]-2-thieny1]-2-thieny1]-2-thieny1]-2-thieny1]-2-thieny1]-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-2,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-2-thieny1]-3-(dicyanomethylene)-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-2-methyl-3,5-dihydro-3,5-dihyd

Double bond geometry as shown.

PAGE 1-A

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

701235-59-8 CAPLUS Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-, 3-[4-cyano-3-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]beneyl]-2-thienyl]popyl ester (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-B

701235-61-2 CAPLUS 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-

[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-2-[3-[[4-[(1,2,2-trifluoroethenyl)oxy]benzoyl]propyl]-3-furanyl]ethenyl]-2-thienyl]benzoyl]benzoyl]benzoyl]benzoyl]benzoyl]benzoyl]ethenyl]benzoyl]

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

PAGE 2-B

RN 701235-63-4 CAPLUS CN 1,2-Benzenedicarboxylic acid, 1-[6-[[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[2-[3-

[[3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propy
[3,1-4-cyano-5-(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]ethylamino]hexyl] ester (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued) PAGE 1-A

PAGE 1-B

L65 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:970715 Document No. 141:164293 Simple reflection measurement of
nonlinear optical activity using silicon as an electrode. Haller, Marnie
A.; Lawson, Rhys; Clot, Olivier; Sherwood, Travis; Dalton, Larry; Jen,
Alex K. (Department of Materials Science and Engineering, Univ. of
Washington, Seatle, WA, 98195, USA). Proceedings of SPIE-The
International Society for Optical Engineering, 5212 (Linear and Nonlinear
Optics of Organic Materials III), 226-331 (English) 2003.
CODEN: PSISO. ISSN: 0277-786X. Publisher: SPIE-The International
Society for Optical Engineering.
AB Future generations of photonic devices which incorporate poled organic
nonlinear optical materials may be aided by, or require the use of
non-traditional electrodes. This report details the integration of
highly
doped Si as one of the poling/modulating electrodes in the simple
reflection type experiment for determination of nonlinear optical
activity in a

reflection type experiment --- activity in a guest-host polymer system. The measurements illustrate that the behavior of doped-Si and the traditional In Sn oxide (ITO) electrodes are analogous. A number of organic chromophore guests were studied as well

multiple polymer hosts. Results demonstrate both successful poling and subsequent modulation of NLO materials, including the calcn. of r33 values

IT

es comparable to those achieved using a standard ITO electrode. 729612-75-3 RL: PRP (Properties) (simple reflection measurement of nonlinear optical activity using silicon as electrode) 729612-75-3 CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-(dieth)]amino)]heny]|ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:939698 Document No. 141:133276 Novel fluorophores for single-molecule imaging. Willets, Katherine A.; Ostroverkhova, Oksana; Hess, Stephan;

Meng; Twieg, Robert J.; Moerner, William E. (Department of Chemistry, Stanford Univ., Stanford, CA, USA). Proceedings of SPIE-The

Society for Optical Engineering, 5222(Nanocrystals, and Organic and

Nanomaterials), 150-157 (English) 2003. CODEN: PSISDG. ISSN: 0277-786X. Publisher: SPIE-The International Society for Optical

0277-786X. Publisher: SPIE-The International Society for Optical Engineering.
A new class of fluorophores has been identified that can be imaged at the single-mol. level and offer addnl. beneficial properties such as a significant ground state dipole moment, moderate hyperpolarizability, and sensitivity to local rigidity. These mols. contain an amine donor and a dicyanodihydrofuran (DCDHF) acceptor linked by a conjugated unit zene.

dicyanounyututuan (became)
(benzene,
thiophene, alkene, styrene, etc.) and were originally designed to deliver
both high polarizability anisotropy and dipole moment as nonlinear

six

dyes in this new class of single-mol. reporters, with absorption maxima ranging from 486 to 614 nm.

IT 500198-25-4
RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(Fluorophores based on dicyanodihydrofuran acceptors paired with amine donors for single-mol. imaging)
RN 500198-25-4 CAPFUS
CN Propanedinitrile,
2-[3-cyano-4-[2-[5-(dihexylamino)-3-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:855295 Document No. 139:3558790 Low loss electro-optic polymers and devices made therefrom. He, Mingqian; Shustack, Paul J.; Wang, Jianguo (USA). U.S. Pat. Appl. Publ. US 20030201429 Al 20031030, 21 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-136869 20020430.

An electro-optic chromophore is described comprising a compound having a general formula I, wherein  ${\tt D}$  = an electron donor having one or a AB

plurality
of terminally pendent, polymerizable cyclic ether or cyclic thioether
groups; B = at least one bivalent aromatic ring or derivs.; and R2 and

(each, independently) H, or a (un)substituted C1-C10 alkyl, a (un)substituted C2-C10 alkenyl, a (un)substituted aryl, a (un)substituted alkylaryl, a (un)substituted carbocycle, a (un)substituted heterocycle,

a (un)substituted cyclohexyl; or R2 and R3 together form a (substituted) ring structure. The chromophore may have nonlinear optical property and may be photocurable. An optical device using the chromophore is also described. A method of fabricating an optical or electro-optic structure containing a photodefinable high  $\mu\beta$  chromophore layer is also described. lescribed TT

described. 618439-10-4P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);

(Reactant or reagent)

(Reactant or reagent)
(chromophore; low loss electro-optic polymers and devices using them)
(618439-10-4 CAPLUS
Propanedinitrile,
-cyano-5-(4-cyclohexylphenyl)-4-[2-[3,4-dihexyl-5-[2-[4-[methyl]-2-oxianylmethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5methyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 - \text{N} \\ \text{CH} = \text{CH} \\ \text{CH} = \text{CH} \\ \text{CH}_2)_5 \\ \text{(CH}_2)_5 - \text{Me} \\ \text{NC} \\ \text{CN} \\ \end{array}$$

L65 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:801303 Document No. 140:17234 Novel chromophore-functionalized
poly[2-(trifluoromethyl)adamentyl acrylate-methyl vinyl urethane]s with
high poling stabilities of the nonlinear optical effect. Briers, David;
Koeckelberghs, Guy; Picard, Isabel; Verbiest, Thierry, Persoons, Andre;
Samyn, Celest (Laboratory of Macromolecular and Physical Organic
Chemistry, Katholieke Universiteit Leuven, Heverlee, 3001, Belg.).
Macromolecular Rapid Communications, 24(14), 841-846 (English)
2003. CODEN: MRCOEJ. ISSN: 1022-1336. Publisher: Wiley-VCH
Verlag GmbH & Co. KGAA.
AB Nonlinear optical vinyl polymers with high glass transition temperature
(Tg)

were prepared by the functionalization of a fluorinated acrylate-Me vinyl isocyanate copolymer. A modified pathway to obtain a thiophene bridged chromophore was worked out. Poled films of the polymers show a fairly high and stable nonlinear optical response, even at elevated temps. 629649-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (in prepas. of thiophene-bridged chromophore mols. for synthesis of adamantyl- and urethane-bearing acrylate polymers having nonlinear optical effects) 629649-92-9 CAPLUS
Propanedinitriie, 2-[3-cyano-4-[2-[5-[(1E)-2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

629649-92-9DP, reaction product with adamantyl- and isocyanate-bearing polyacrylates and alcs. RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Reactant or reagent)
(synthesis of chromophore-functionalized adamantyl- and urethane-bearing acrylate polymers having nonlinear optical effects)
629649-92-9 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[(1E)-2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

L65 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:756534 Document No. 140:34537 Focused microwave-assisted synthesis of
2,5-dihydrofuran derivatives as electron acceptors for highly efficient
nonlinear optical chromophores. Liu, Sen; Haller, Marnie A.; Luo,
Jingdong; Jang, Sei-Hum; Ma, Hong; Dalton, Larry R.; Jen, Alex K.-Y.
(Departments of Materials Science and Engineering and Chemistry,
University of Washington, Seattle, WA, 98195, USA). Materials Research
Society Symposium Proceedings, 771 (Organic and Polymeric Materials and
Devices), 375-380 (English) 2003. CODEN: MRSPDH. ISSN:
0272-9172. Publisher: Materials Research Society.

AB A diversified family of 2,5-dihydrofuran derivs. has been synthesized as

new class of highly efficient and tunable electron acceptors using the single-mode focused microwave irradiation. High poling efficiency and

large electro-optic coeffs. (r33 values of 128 and 116 pm/V at 1.3  $\mu$ m) have been demonstrated using 2-dioyanomethylene-3-cyano-4,5-dimethyl-5-trifluoromethyl-2,5-dihydrofuran (CF3-TCF)-based chromophores as dopant

poly(Me methacrylate) (FMMA) and a high glass-transition temperature polyquinoline (PQ-100) resp. Films were doped with

[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadienyl]-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]propanedinitrile.

Excellent

llent dipole alignment stability has also been demonstrated in the guest/host composite at 85°C. Multi-functionalized NLO chromophores based on hydroxy containing 2,5-dihydrofuran acceptors were also synthesized

ugh
microwave methodol. for further characterizations.
613237-39-1, [3-Cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4(dibutylamino)phenyl]-1,3-butadienyl]-2-thienyl]ethenyl]-5-methyl-5(trifluoromethyl)-2[5H)-furanylidene]propanedinitrile
613237-40-4, [3-Cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4(dibutylamino)phenyl]-1,3-butadienyl]-4-[[[(1]dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5(trifluoromethyl)-2[5H)-furanylidene]propanedinitrile
613237-41-5, [3-Cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4(dibutylamino)phenyl]-1,3-butadienyl]-2-thienyl]ethenyl]-5,5-dimethyl2(5H)-furanylidene]propanedinitrile
613237-42-6,

[3-Cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadienyl]4-[[(1,1-dimethylethyl)dimethyleilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5dimethyl-2(5H)-furanylidene]propanedinitrile
RL: PRP (Properties)
(focused microwave-assisted synthesis of dihydrofuran derivs. as
electron acceptors for highly efficient nonlinear optical

electron acceptants for any and acceptant and acceptant and acceptant and acceptant acceptant and acceptant acceptan

Double bond geometry as shown.

L65 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

613237-40-4 CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[(1,1-dimethylathyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

613237-41-5 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-y1]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

 $613237-42-6 \quad CAPLUS \\ Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[(1,1-dimethylatiyl)dimethylsilylloxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)$ 

L65 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Me 
$$(CH_2)_5$$
  $Me$   $(CH_2)_5$   $Me$   $(CH_2)_5$ 

RN 676256-53-4 CAPLUS
Propanedinitrile,
2-[3-cyano-4-[(1E)-2-[3,4-diethyl-5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown

676256-54-5 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3,4-dipropyl-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 676256-55-6 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[(1E)-2-[3,4-dibutyl-5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:632276 Document No. 140:294194 Effects of alkyl spacer group length on
Vis-NIR absorption behavior in FTC-like guest-host EO polymers. Barto,
Richard R., Jr.; Bedworth, Peter V.; Epstein, Joseph A.; Ermer, Susan P.;
Taylor, Rebecca E.; Frank, Curtis W. (Lockheed Martin Space Systems Co.,
USA). Proceedings of SFIE-The International Society for Optical
Engineering, 4991 (Organic Photonic Materials and Devices V), 575-588
(English) 2003. CODEN: PSISDG. ISSN: 0277-786X. Publisher:
SPIE-The International Society for Optical Engineering,
AB Spectral absorption behavior of FTC-like dyes of varying shape
incorporated into amorphous polycarbonate (ARC) were characterized by
photothermal deflection spectroscopy. Previous Monte Carlo calcns. by
Dalton and Robinson predict a strong dependence of the macroscopic
nonlinear optical susceptibility on the chromophore waist:length aspect
ratio in elec. field-poled films. This dependence arises from London
interactions between chromophores, which are expected to influence the
absorption characteristics of the composite both by changing the local
polarity of the medium and through dipole interactions. It is expected
that these interactions will play a role in the absorption
characteristics

of unpoled films as well. Of particular interest are the spectral
characteristics of the red edge of the main dye electronic absorption
peak, and the fine structure in the near-IR, dominated by overtones of
fundamental C-H stretching and bending modes. The spectral structure in
these key regions can be influenced by inter- and intramol. interactions
and conformational changes in the dye. The near-IR structure, in turn,
will dictate absorption loss in optical devices prepared from these
materials at key transmission wavelengths (1.3 and 1.55 µm). A
homologous series of spacer lengths, ranging from Et to heavl, attached to

an FTC-like NLO chromophore, LMCO-46M, was characterized by a combination of photothermal deflection spectroscopy (PDS) and UV-visible spectroscopy to examine the effects of the mol. environment on near-IR loss at 1090

nm,

1300 nm and 1550 nm. 473796-78-0 676256-53-4 676256-54-5 473796-78-0 676256-55-6

:256-55-6 : COU (Occurrence, unclassified); PRP (Properties); OCCU (Occurrence) (effects of alkyl spacer group length on Vis-NIR absorption behavior RL: OCU in

FTC-like guest-host EO polymers)

#1736-79-0 CAPLUS # POPLING # POPLIN

Double bond geometry as shown.

L65 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

Me Me Me 
$$Me$$
  $CN$   $CN$   $CN$ 

L65 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:454741 Document No. 139:439920 Second order nonlinear optical
chromophores containing a donor and an acceptor part linked by a
π-bridge including a substituted thiophene ring; and electrooptical
devices employing the chromophores. Huang, Diyun; Chen, Baoquan (Lumera
Corp., USA). U.S. Pat. Appl. Publ. U.S 2003107027 Al 20030612,
15 pp., Cont.-in-part of U.S. Ser. No. 932,831. (English). CODEN:
USXXCO. APPLICATION: US 2002-301978 20021122. PRIORITY: US
2000-PV226267

20000817; US 2001-932831 20010817. GT

Nonlinear optical chromophores are described by the general formula I where, independently at each occurrence: R1 is absent or a  $\pi$ -bridge; R2 is absent or a  $\pi$ -bridge; D is a donor; A is an acceptor; X is O or S; and R is an alkyl, aryl, heteroalkyl, or heteroaryl group. Nonlinear optical chromophores having the formula D- $\pi$ -A are also described, where  $\pi$  is a  $\pi$ -bridge including a thiophene ring having O atoms bonded directly to the 3 and 4 positions of the thiophene ring, D is a donor,

A is an acceptor. Second order nonlinear optical compns. comprising a polymer matrix and the nonlinear chromophores are also discussed as are electrooptical devices comprising the nonlinear optical compns. 540777-76-2P 540777-77-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (second-order nonlinear optical chromophores containing donor and

IT

acceptor , parts linked by  $\pi ext{-bridge}$  including substituted thiophene prepared

using) 540777-76-2 CAPLUS

Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutoxy-2thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

540777-78-4P 540777-78-4P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)
(second-order nonlinear optical chromophores containing donor and

ptor

parts linked by \$\pi\$-bridge including substituted thiophene; and electrooptical devices employing chromophores)
540777-78-4 CAPLUS
Benzoic acid, 4-[(trifluoroethenyl)oxy]-,
[[4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl]-2-thienyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl]ethenyl[ethenyl[ethenyl]ethenyl[e

Double bond geometry as shown.

L65 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

540777-77-3 CAPLUS
Propanedinitrile, 2=[4-[(1E)-2-[5-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]=thenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3,9-dimethyl-2(5H)-furanylidene]-

(CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A n-BuO OBu-n n-BuO `OBu−n

PAGE 1-B

540777-74-0P

RI: PEF (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); SUSES (Uses) (second-order nonlinear optical chromophores containing donor and

ports linked by π-bridge including substituted thiophene; and electrooptical devices employing chromophores) 540777-74-0 CAPLUS 540777-74-0 CAPLUS Propanedinitrile, 2-[3-q-ano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethyl-lamino)phonyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-Furanylidene]- (CA INDEX NAME)

L65 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

586972-36-3P 586972-37-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chromophore; chiral helical chromophore-functionalized polybinaphthalenes synthesis)
586972-36-3 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl(2-hydroxyethyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

CAPLUS

S069/2-3/-4 CAPLUS = (3-cyano-4-[2-[5-[2-[4-[ethy1(6-hydroxyhexyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene|- (CA INDEX NAME)

L65 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:421608 Document No. 139:214850 Synthesis and properties of chiral
helical chromophore-functionalized polybinaphthalenes for second-order
nonlinear optical applications. Koeckelberghs, Guy, Sioncke, Sonja;
Verbiest, Thierry; Persoons, Andre; Samyn, Celest (Laboratory of
Macromolecular and Physical Organic Chemistry, Katholieke Universiteit
Leuven, Heverlee, B-3001, Belg.). Polymer, 44(14), 3785-3794 (English)
2003. CODEM: POLMAG. ISSN: 0032-3861. Publisher: Elsevier
Science Ltd..

Science Ltd..
Chiral, helical, nonlinear optical polybinaphthalenes were prepared by covalent bonding of chromophores to the backbone of polybinaphthalenes

a Mitsunobu reaction. This was achieved in a two-step reaction, with the formation of a precursor polymer by a Suzuki coupling reaction, which was afterwards functionalized with chromophores. It was tried to achieve a chiral ordering of the chromophores by attaching them to a chiral,

chiral ordering of the chromophores by attaching them to a chiral, helical polymer backbone. Poled films of the polymers were measured for their second-harmonic generation effect and showed nonresonant nonlinear susceptibilities (yzzr(2)(0)) up to 10.6 pm/V.

IT 586972-36-3DP, reaction product with chiral polybinaphthalenes 586972-37-4DP, reaction product with chiral polybinaphthalenes RL: PRP (Properties); SPN (Synthetic preparation); PREF (Preparation) (chiral helical chromophore-functionalized polybinaphthalenes synthesis)

RN 586972-36-3 CAPLUS

CN Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl (2-hydroxyethyl)amino]phenyl]etenyl]-2-thienyl]etenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

586972-37-4 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[ethyl(6-hydroxyhexyl)amino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:402555 Document No. 139:124648 High-performance photorefractive
organic
glass with near-infrared sensitivity. Ostroverkhova, Oksana; Moerner, W.
E.; He, Meng; Twieg, Robert J. (Department of Chemistry, Stanford
University, Stanford, CA, 94305-5080, USA). Applied Physics Letters,
82(21), 3602-3604 (English) 2003. CODEN: APPLAB. ISSN:
0003-6951. Publisher: American Institute of Physics.
AB A high-performance organic glass mixture comprised of two
dicyanomethylenedihydrofuran derivs. is presented. A pronounced two-beam
coupling effect was observed at a wavelength of 830 nm in an unsensitived
composition Sensitization with
(2,4,7-trinitro-9-fluorenylidene)malononitrile
(TNFM) led to a significant increase in the two-beam coupling gain
coefficient,
reaching a net value of .apprx.370 cm-1 at an elec. field of 45 V/µm at
18 TNFM, and resulted in an improvement in photorefractive speed.
R1. PRP (Properties)
(high-performance photorefractive organic glass with near-IR
sensitivity

(high-performance procests
sensitivity
and its properties)
RN 551291-76-7 CAPLUS
CN Propanedinitrils
2-[3-cyano-4-[2-[5-(dihexylamino)-2-thienyl]ethenyl]-5,5dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2003:338986 Document No. 139:3233820 Focused microwave-assisted synthesis

2,5-dihydrofuran derivatives as electron acceptors for highly efficient nonlinear optical chromophores. Liu, Sen; Haller, Marnie A.; Ma, Hong; Dalton, Larry R.; Jang, Sei-Hum; Jen, Alex K.-Y. (Department of Materials Science and Engineering, University of Washington, Seattle, WA, 98195-2120, USA). Advanced Materials (Weinheim, Germany), 15 (7-8), 603-607 (English) 2003. CODEN: ADVMEM. ISSN: 0935-9648. OTHER SOURCES: CASREACT 139:323382. Publisher: Wiley-VCH Verlag GmbH & Co. KGAA.

GT

 $\ensuremath{\mathsf{AB}}$  A very diversified family of 2,5-dihydrofuran derivs., e.g., I, was prepared

ured as a new class of tunable electron acceptors using single-mode focused microwave irradiation A high poling efficiency and very large r33

es (128 and 116 pm V-1 at 1.3 µm) were demonstrated using I in polymethyl methacrylate and a high-temperature polyquinoline (PQ-100). An excellent long-term temporal stability was demonstrated in the PQ guest/host

long-term temporal stability was demonstrated...

system.

IT 613237-39-1P 613237-40-4P 613237-41-5P

RL: MOA (Modifier or additive use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(focused microwave-assisted synthesis of 2,5-dihydrofuran derivs. as electron acceptors for nonlinear optical chromophores)

RN 613237-39-1 CAPLUS

CN Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) dimethylethyl)dimethylsilyl)oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

 $\begin{array}{lll} 613237-40-4 & CAPLUS \\ Propanedinitriile, & 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[[(1,1-dimethylatinyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5-methyl-5-(trifluoromethyl)-2(5H)-furanylidene]- & (CA INDEX NAME) \\ \end{array}$ 

Double bond geometry as shown.

613237-41-5 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4-(dibutylamino)phenyl]-1,3-butadien-1-y1]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene)- (CA INDEX NAME)

Double bond geometry as shown.

613237-42-6P

613237-42-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(focused microwave-assisted synthesis of 2,5-dihydrofuran derivs. as
electron acceptors for nonlinear optical chromophores)
613237-42-6 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E,3E)-4-[4(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[(1,1-

L65 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2003:301346 Document No. 138:322077 Crosslinkable monomers for novel nonlinear optical polymers. Yu, Luping (The University of Chicago,

POTI Int. Appl. W0 2003032072 A2 20030417, 58 pp. DESIGNATED
STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, RG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, CM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SI, TJ, TM, TH, TT, TZ, UA, UG, UZ, VN, VT, ZA, ZM, ZW; RN: AT, BE, BF, BJ, CF, CG, CH, CI, CK, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.
(English). CODEN: PIXXDZ. APPLICATION: WO 2002-US22531 20020715.
PRIORITY: US 2001-PV305374 2010713.
Novel compns. and synthetic methods for forming nonlinear optic polymers, which may be incorporated into multiple light-based devices, are disclosed. These compns. include crosslinkable chromophoric monomer s

units

disclosed. These compns. include crosslinkable chromophoric monomers that incorporate nonlinear optic chromophores, linking monomers that may be used to link chromophoric monomers, and polymers made from crosslinkable chromophoric monomers or chromophoric monomers in combination with linking monomers. The polymers can exhibit high thermal stability, which is believed to arise from their covalently bonded chromophore structures. In one aspect, linking monomers are disclosed that may be crosslinked.

488809-62-TP
RL: IMF (Industrial manufacture); PREP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(monomers; synthesis of crosslinkable monomers for novel nonlinear optical polymers)

488809-62-T CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-

dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

511535-61-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting materials; synthesis of crosslinkable monomers for novel
nonlinear optical polymers)
511535-61-8 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[3-[2,5-bis[[1,1-

dimethylethyl) dimethylsilyl]oxy]phenyl]propyl]methylamino]phenyl]ethenyl]2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX

L65 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

488809-63-8P IT

400003-03-01 RI: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (synthesis of crosslinkable monomers for novel nonlinear optical

polymers) 488809-63-8 CAPLUS

NN 4050U3-03-8 CAPLUS
CN Benzoic acid,
4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(1,3dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)]bis-, polymer with
[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-

dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]propanedinitrile (9CI) (CA INDEX NAME)

CM 1

CRN 488809-62-7

L65 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2003:58363 Document No. 138:1232760 Nonlinear optical polymers, compositions, and their manufacture. Yu, Luping (The University of Chicago, USA). PCT Int. Appl. Wo 2003007071 A2 20030123, 66 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ

DESIGNATED STATES: W: AE, AG, AL, AM, AT, AN, AZ, BA, BB, BG, BK, BY,
CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE,
GH, CM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
LT, LU, LV, MA, MD, MG, MK, MN, MM, MM, MZ, NO, NZ, CM, PH, FL, PT, RO,
RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, VU,
ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RM: AT, BE, BF, BJ, CF,
CG, CH, CI, CM, CY, DE, DR, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML,
MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.
APPLICATION: WO 2002-US22533 20020715. PRIORITY: US 2001-PV305374
20010713.

These compns. include chromophoric monomer units that incorporate
nonlinear optic chromophores, linking monomers that may be used to link
chromophoric monomers, and polymers made from chromophoric monomers or
chromophoric monomers in combination with linking monomers. The polymers
can exhibit high thermal stability, which is believed to arise from their
covalently bonded chromophore structures. In addition to their

covalently bonded chromophore structures, nonlinear optic polymers may be crosslinked

dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]propanedinitrile (9CI) (CA INDEX NAME)

CM 1

CRN 488809-62-7 CMF C34 H30 N4 O3 S

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH} \\$$

L65 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN CMF C34 H30 N4 O3 S (Continued)

CM 2

L65 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN CRN 133532-50-0 CMF C33 H16 F6 N2 O8 (Continued)

CM 1

CRN 488809-62-7 CMF C34 H30 N4 O3 S

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ANSWER 16 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

3:58362 Document No. 138:128790 Novel nonlinear optical polymers
incorporating amines. Yu, Luping (The University of Chicago, USA). PCT
Int. Appl. No 2003001707 Al 20030123, 68 pp. DESIGNATED STATES:
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO,
CR, CU, CZ, DE, DK, DM, CD, EC, EE, ES, FI, GB, GB, GH, CM, HR, HU,
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MM, MG, MK, NM, MM, MX, MZ, NO, NZ, CM, PH, FL, FT, FO, EU, SD, SE, SG,
SI, SK, SL, TJ, TM, IN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, BU, TJ, TM, EW: AT, BE, BF, BJ, CF, CG, CG, CI, CI,
CW, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, FT,
SS, SN, DT, TG, TR. (English). CODEN FIXXD2. APPLICATION: WO
2002-US22532 20020715. PRIORITY: US 2001-305374P 20010713.
Compds. for forming nonlinear optical polymers are described by the
general formula X-Y-Z, (X = (RI-O-CH2-CH2-)2N-; RI = a labile group; Y is
a thiphene oligomer terminated with attached to X via a 1,4-phenylene
bridge; Z= is an electron-withdrawing group; and Y and Z in combination
form a nonlinear optical chromophore). Polymerization of the compds. to
                       polymers, the polymers formed from the compds., and electrooptical
 devices using them)
RN     48889-63-8     CAPUS
CN     Benzoic acid,
4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(1,3-
dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)]bis-, polymer with
[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-
 dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-
dimethyl-2(5H)-furanylidene]propanedinitrile (9CI) (CA INDEX NAME)
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L65 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:58361 Document No. 138:123275 Nonlinear optical polymers,
compositions,
and their manufacture. Yu, Luping (The University of Chicago, USA). Pi
Int. Appl. NO 2003007069 A2 20030123, 81 pp. DESIGNATED STATES:
W: AE, AG, Al, AM, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO,
CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LK, LE, LI, LI, LV, LV,
AM, MD, MG, MK, MN, MN, MX, MZ, NO, NZ, CM, PH, PL, FT, RO, RU, SD, SE, SG,
SI, SK, SL, IJ, IM, IN, IR, IT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZM, ZW,
AT, BE, BF, BJ, CF, CG, CH, C1, CM, CY, DE, DK, ES, FI, FR, GA, GB, GE,
IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English).
CODER: PIXXD2 APPLICATION: NO 2002-US22376 20020715. PRIORITY: US
2001-PV305374 20010713. USA). PCT

These compns. include chromophoric monomer units that incorporate nonlinear optic chromophores, linking monomers that may be used to link chromophoric monomers, and polymers made from chromophoric monomers or chromophoric monomers in combination with linking monomers. The polymers can exhibit high thermal stability, which is believed to arise from their covalently bonded chromophore structures. In addition to their AB

covalently bonded chromophore structures, nonlinear optic polymers may be crosslinked

slinked to further increase the thermal and dipole stability of the polymers. Thus, monomer I having electron withdrawing group Q (3-(dicyanomethylene)-2,3-dihydrobenzo[b]thiophene) (preparation given)

polymerized with the diacid II to give polyester polyimide having a  $\lambda max709,$  glass transition temperature 170°, and decomposition

488809-63-8P

488809-63-8P
RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)
(nonlinear optical polyester polyimide manufacture and property)
488809-63-8 CAPLUS
Benzoic acid,
-[[2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(1,3-didyaco-2H-isoindole-5,2-diyl)]bis-, polymer with
[3-cyano-4-[2-[5-[2-[4-[[3-(2,5-

dihydroxyphenyl)propyl]methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]propanedinitrile (9CI) (CA INDEX NAME)

CRN 488809-62-7 CMF C34 H30 N4 O3 S

L65 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CRN CMF 133532-50-0 C33 H16 F6 N2 O8

L65 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

2  ${\tt CM}$ 

CRN 133532-50-0 CMF C33 H16 F6 N2 O8

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dendron synthesis; design, synthesis, and properties of highly efficient side-chain dendronized nonlinear optical polymers for electro-optics)
RN 502449-13-0 CAPLUS
CN Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-, 3-[4-cyano-5-(dicyanomethylene)-3-[2-[5-[4-[4-[ethyl][6-

(methoxymethoxy)hexyl]amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]2,5-dihydro-2-methyl-2-furanyl]propyl ester (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{CF2} \\ \text{F-C-O} \\ \text{CH2} \\ \text{NC-CH2} \\ \text{NC-CH2} \\ \text{NC-CH2} \\ \text{CH2} \\ \text{O-C-F} \\ \text{CH2} \\ \text{CH2} \\ \text{O-C-F} \\ \text{CH2} \\ \text{O-C-F} \\ \text{CH2} \\ \text{CH3} \\ \text{CH3}$$

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2003:3036 Document No. 138:255621 Design, synthesis, and properties of
highly efficient side-chain dendronized nonlinear optical polymers for
electro-optics. Luo, Jindong; Liu, Sen; Haller, Marnie; Liu, Lu; Ma,
Hong; Jen, Alex K.-Y. (Department of Materials Science and Engineering,
University of Washington, Seattle, WA, 98195-2120, USA). Advanced
Materials (Weinheim, Germany), 14(23), 1763-1768 (English) 2002.
CODEN: ADVMEW. ISSN: 0935-9648. Fublisher: Wiley-VCH Verlag GmbH & Co.
KGAA.

(methoxymethoxy)hexyl]amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]5-(3-hydroxypropyl)-5-methyl-2(5H)-furanylidene)- (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

502449-13-0P 502449-15-2P

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

502449-15-2 CAPLUS
Benzoic acid, 3,5-bis[[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]-,
3-[4-cyano-5-(dioyanomethylene)-3-[2-[5-[4-[4-[ethyl(6-hydroxyheyl)amino]phenyl]-1,3-butadien-1-[4-[4-[ethyl]ethenyl]-2,5-dihydro-2-methyl-2-furanyl]propyl ester (CA INDEX NAME)

PAGE 1-A

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A I— (СН<sub>2</sub>)<sub>6</sub>—ОН

T 502449-17-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dendron; design, synthesis, and properties of highly efficient side-chain dendronized nonlinear optical polymers for electro-optics)
RN 502499-17-4 CAPLUS
CN 1,2-Benzenedicarboxylic acid,
1-[6-[4-[4-[5-[2-2-3-[15,5-bis:[4-[(1,2,2-trifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester (CA INDEX NAME)

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) dendronized nonlinear optical polymers for electro-optics)
RN 502558-65-8 CAPLUS
CN Phenol, 4-ethenyl-, homopolymer,
6-[[4-[4-[5-[2-2]-2]-3-[13,5-bis[[4-[(1,2,2-tifluoroethenyl)oxy]phenyl]methoxy]benzoyl]oxy]propyl]-4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butadien-1-yl]phenyl]ethylamino]hexyl 1,2-benzenedicarboxylate 4-[(1,2,2-trifluoroethenyl)oxy]benzoate (CA INDEX NAME)

CM 1

PAGE 1-A CF<sub>2</sub>

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A CF<sub>2</sub>

502558-65-8P 502558-70-5P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (design, synthesis, and properties of highly efficient side-chain IT

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

CM CRN 134151-66-9 CMF C9 H5 F3 O3

CM 3

CRN 24979-70-2 CMF (C8 H8 O)x CCI PMS

CM 4

CRN 2628-17-3 CMF C8 H8 O

502558-70-5 CAPLUS Phenol, 4-ethenyl-, homopolymer, benzoate

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
6-[[4-[4-[5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]-1,3-butdadien-1-yl]phenyl]ethylamino]hexyl
1,2-benzenedicarboxylate (CA INDEX NAME)

CM 1

CRN 502449-25-4 CMF C42 H40 N4 05 S

PAGE 1-B

CM 2

CRN 65-85-0 CMF C7 H6 O2

см з

CRN 24979-70-2 CMF (C8 H8 O)x CCI PMS

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
highly efficient side-chain dendronized nonlinear optical polymers for
electro-optics)
RN 502449-21-0 CAPLUS
CN Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl(6hydroxyhexyl)amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5,5dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

— CM

502449-25-4P 502449-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pendent chromophore; design, synthesis, and properties of highly efficient side-chain dendronized nonlinear optical polymers for electro-optics)
502449-25-4 CAPLUS
1,2-Benzenedicarboxylic acid, 1-[6-[[4-[4-[5-[2-[4-cyano-5-

(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]ethenyl]-2-thienyl]1,3-butadien-1-yl]phenyl]ethylamino]hexyl] ester (CA INDEX NAME)

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

> CRN 2628-17-3 CMF C8 H8 O

502449-23-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(pendent chromophore synthesis; design, synthesis, and properties of
highly efficient side-chain dendronized nonlinear optical polymers for
electro-optics)
502449-23-2 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-[ethyl]6-

(methoxymethoxy)hexyl]amino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

502449-21-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (pendent chromophore synthesis; design, synthesis, and properties of

L65 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

L65 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002:833542 Document No. 137:332023 Highly hyperpolarizable chromophore for core guest host systems useful for electro-optic devices. Taylor,

ca Ellen; Ermer, Susan Patricia; Bedworth, Peter V.; Lovejoy, Steven M.; Leung, Doris S.; Warren, Hope B. (USA). U.S. Pat. Appl. Publ. US 20020161165 A1 20021031, 3 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-119316 20010410.

AB A chromophore in a polymer is given having the structure I in a polyoarbonate matrix. The composition is useful for electro-optic material

rial that does not suffer (by heat) from the limitations of prior materials used in the art. It is a further object to provide a new class of highly hyperpolarizability organic chromophores. It is yet a further object of

invention to show a process for synthesizing the novel highly hyperpolarizable organic chromophores. Another object is to provide

ses such as electrooptical modulators employing the new class of novel highly hyperpolarizable organic chromophores. 473796-78-0P RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) 473796-78-0P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(chromophore; highly hyperpolarizable chromophore for core guest host systems useful for electro-optic devices)
473796-78-0 CAPLUS
Propapadia:

systems userul for electro-open actions, 47376-78-0 CAPLUS 47376-78-0 CAPLUS Propanedinitrile, 2=[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002:787053 Document No. 138:14286 Synthesis of Chromophores with Extremely High Electro-optic Activities. 2. Isophorone- and Combined Isophorone-Thiophene-Based Chromophores. He, Mingqian; Leslie, Thomas

M.; Sinicropi, John A.; Garner, Sean M.; Reed, Leon D. (Corning Incorporated, Corning, NY, 14831, USA). Chemistry of Materials, 14(11), 4669-4675 (English) 2002. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.
AB Four new isophorone and combined isophorone and thiophene bridged chromophores have been synthesized. All of these new high μβ chromophores possess our newly synthesized tricyanovinyldihydrofuran acceptors. Because of our unique acceptor design, all of our chromophores show high solubility in all organic solvents due to minimized chromophore-chromophore electrostatic interactions. These chromophores have also been studied with respect to their solvatochromism and thermal behavior by TGA in air. Freliminary EO characterization of one of these chromophores in polycarbonate has demonstrated an extremely high r33 of

pm/V at 1550 nm. We believe that this is the largest r33 reported at

this

477741-17-6P

477741-16-5P 477741-17-6P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis of isophorone- and combined isophorone-thiophene-based chromophores with extremely high electro-optic activities) CAPLUS

Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[2-[5-[[3-[2-[4-

(diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]methyl]3,4-dihexyl-2-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} & \text{Me} \\ \text{NC} & \text{CH} \\ \text{O} \\ \text{D} \\ \text{D} \\ \text{Me} \\ \text{Me} \\ \end{array}$$

477741-17-6 CAPLUS Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[2-[5-[3-[3-[2-[4-

L65 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) (diethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]-1-

PAGE 1-A

L65 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002:787052 Document No. 138:246080 Synthesis of Chromophores with

2002.787052 Document No. 138:246080 Synthesis of Chromophores with Extremely

High Electro-optic Activity. 1. Thiophene-Bridge-Based Chromophores. He, Mingqian; Leslie, Thomas M.; Sinicropi, John A. (Corning Incorporated, Corning, NY, 14831, USA). Chemistry of Materials, 14(11), 4662-4668 (English) 2002. COURN: CMATEX. ISSN: 0897-4756. OTHER SOURCES: CASRECT 138:24608. Publisher: American Chemical Society.

AB We have successfully synthesized several new substituted thiophene-based electro-optic chromophores. All of these chromophores have structures similar to FTC but they incorporated our newly designed tricyanovinyldhydrofuran acceptors. Since these acceptors possess an anisotropic structure, all of the chromophores are very soluble in a wide range of organic solvents. Thermal study of these chromophores by TGA shows

all of them are very stable in air. UV spectra indicate the chromophores by IoA s all of them are very stable in air. UV spectra indicate the chromophores have a large solvatochromic effect, implying very large mol. nonlinearities.

477892-06-1P 477892-32-3P 477892-34-5P 477892-33-6P 477892-33-9P 477892-39-9P 477892-39-9P 477892-40-3P

RL: PRP (Properties); SFN (Synthetic preparation); PREP (Preparation) (chromophore; synthesis of thiophene-bridge-based chromophores with extremely high electro-optic activity)

477892-06-1 CAPLUS

Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl]]-dynaminjphenyl]-thenyl]-4-decyl-2-thienyl]phenyl]idimethylsilyljoxy]ethyljaminojphenyl]-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

477892-32-3 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-dimethyl+hyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(2,4-difluorophenyl)-5-methyl-2(5H)-

hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown

477892-36-7 CAPLUS Propanedinitrile, 2-[4-[(1E,3E)-4-[5-[(1E)-2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dihexyl-2-

thienyl]-1,3-butadien-1-yl]-3-cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN furanylidene]- (CA INDEX NAME) (Continued)

Double bond geometry as shown.

477892-34-5 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E,3E)-4-[4-[bis(2-

hydroxyethyl)amino]phenyl]-1,3-butadien-1-yl]-4-decyl-2-thienyl]ethenyl]-3cyano-5-(4-cyclohexylphenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX
NAME)

Double bond geometry as shown.

477892-35-6 CAPLUS

L65 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

RN 477892-37-8 CAPLUS CN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E,3E)-4-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]-1,3-butadien-1-yl]-3,4dihexyl-2-thienyl]ethenyl)-5-(4-butylphenyl)-3-cyano-5-methyl-2(5H)furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

477892-39-0 CAPLUS

CN Propanedinitrile, 2-[3-cyano-5-(4-cyclohexylphenyl)-4-[(1E)-2-[3,4-dihexyl-

 $\begin{array}{lll} 5-[(1E,3E)-4-[4-[(2-hydroxyethyl)methylamino]phenyl]-1,3-butadien-1-yl]-2-thienyl]ethenyl]-5-methyl-2(5H)-furanylidene]-& (CA INDEX NAME) \end{array}$ 

Double bond geometry as shown.

L65 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2002:770496 Document No. 138:97888 Low-voltage electro-optic modulation
using amorphous polycarbonate host material. Ermer, Susan; Lovejoy,
Steven M.; Bedworth, Peter V.; Leung, Doris S.; Warren, Hope B.; Epstein,
Joseph A.; Girton, Dexter G.; Dries, Larry S.; Taylor, Rebecca E.; Barto,
Richard R., Jr.; Eades, Wendell; Van Eck, Timothy E.; Moss, Angelina S.;
Anderson, William W. (Lockheed Martin Advanced Technology Center, Palo
Alto, CA, 94304-1191, USA). Advanced Functional Materials, 12(9),
605-610

 $\mathrm{d}B/\mathrm{c}m,$  which is the confidence limit of the slab measurement used. A Mach-Zehnder modulator fabricated using the push-pull poling technique

has

a low switching voltage (Vm) of 1.2 V.
473796-78-0P, Chromophore 46M
RL: DEV (Device component use); PEP (Physical, engineering or chemical process); PEP (Properties); PYP (Physical process); SPN (Synthetic preparation); PEC (Orpocess); USES (USES)
(Chromophore 46M; low-voltage electro-optic modulation using amorphous polycarbonate host material doped with chromophore 46M)
473796-78-0 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-[ethyl(2-methoxyethyl)amino]phenyl]ethenyl]-3,4-dihexyl-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

477892-40-3 CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dihexyl-5-[(1E)-2-[4-[(2-dydroxyethyl)methylamino]phenyl]ethenyl]-2-thienyl]ethenyl]-5-methyl-5-(2,3,4,5,6-pentafluorophenyl)-2(5H)-furanylidene] (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002;387664 Document No. 136:3874250 Chromophores for polymeric thin films and optical waveguides and devices comprising the same. He, Mingqian; Leslie, Thomas M. (Corning Incorporated, USA). U.S. US 6393190 B1 20020521, 16 pp., Cont.-in-part of U.S. Ser. No. 595,221. (English). CODEN: USXXMA APPLICATION: US 2000-675966 20000929. PRIORITY: US 2000-595221 20000616.

Compds. are claimed which are described by the general formula I (R2 and R3 = rings in which \* denotes a spiro junction or a chiral center; D = electron donating group; B is or contains  $\geq 1$  bivalent aromatic ring; and R2 and R3 = independently selected (un) substituted C1-O alkyl, (un) substituted C2-O alkynyl, (un) substituted d2-O alkynyl, (un) substituted daryl, (un) substituted daryl, (un) substituted carbocyclic, (un) substituted heterocyclic, (un) substituted cyclohexyl, or (CR2)no(CR2)n; and n = 1-10). Methods for preparing the tron-withdrawing

(CH2)no(CH2)n; and n = 1-10). Methods for preparing the electron-withdrawing groups are described. Optical waveguides comprising polymers incorporating the compds., and optical devices (e.g. laser frequency converters, optical interferometric waveguide gates, wideband electrooptical guided wave analog-to-digital converters, and optical parametric devices) incorporating the waveguides, are also described.

IT 383124-87-6P

Jobius-07-07 RI: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (furan derivative chromophores for polymeric thin films and their production

uction
and optical waveguides and devices comprising them)
383124-87-6 CAPLUS
Bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl dichloride,
1,4,5,6,7,7-hexachloro-, polymer with

[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethy1)amino]pheny1]etheny1]-4-decy1-2-thieny1]etheny1]-3-cyano-5-(3,4-dichloropheny1)-5-methy1-2(5H)-furanylidene]propanedinitrile and 2,3,5,6-tetrachloro-1,4-benzenedimethanol (9CI) (CA INDEX NAME)

CRN 383124-85-4 CMF C43 H46 C12 N4 O3 S

Double bond geometry as shown.

L65 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 16673-09-9 CMF C9 H2 C18 O2

CM 3

CRN 7154-26-9 CMF C8 H6 C14 O2

383124-85-4P RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or

L65 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (monomer chromophore; prodn. of intermediates for electrooptical

(monomer chromophore; prodn. of intermediates for electrooptical chromophores)
383124-85-4 CAPLUS
PropanedInitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethylamino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

IT

383124-86-5P RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (monomeric chromophore; production of intermediates for electrooptical

Chromophores)
383124-86-5 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSMER 25 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2002;233700 Document No. 136;2543330 Sterically stabilized second-order
nonlinear optical chromophores and devices incorporating the same.
Dalton, Larry R.; Zhang, Cheng, Wang, Chuanguang; Fetterman, Harold R.;
Wang, Fang; Steier, William; Harper, Aaron W.; Ren, Albert S.; Michael,
Joseph (Pacific Wave Industries, Inc., USA). U.S. US 6361717 B1
20020326, 30 pp., Cont.-in-part of U.S. 6,067,186. (English).
CODEN: USXXAM. APPLICATION: US 2000-488422 20000120. PRIORITY: US
1998-122806 19980277.
AB Nonlinear optical devices are described in which the active element
incorporates a chromophore which includes an electron donor group and an
electron acceptor group joined by a bridge structure, preferably a
ring-locked bridge structure. Preferably, at least the electron acceptor
group is bonded to the bridge structure also includes? I bulky
side group. The bridge structure and complying the preferred embodiment, the bridge structure was comprise two protected alicyclic
rings or ring-locked trienome. Alternately, the chromophore may include
an electron donor group, a ring-locked tricyano electron acceptor group,
and a bridge structure between them. The electron acceptor group may
comprises an isophorone structure. The bridge structure may include a
bithiophene unit or a modified isophorone unit.

IT 351445-08-4 351445-10-8
RI: DEV (Device component use); USES (Uses)
(nonlinear optical chromophores)

(nonlinear optical devices employing sterically stabilized second-order nonlinear optical chromophores)

RN 351445-00-4 CAPLUS

CN Propanedinitrial

2-[3-cyano-4-[2-[5'-[2-[4-(diethylamino)phenyl]ethenyl]-3,3'\*-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

351445-10-8 CAPLUS
Propanedinitrile, 2-[4-[2-[5'-[[6-[2-[4-[bis[2-[[(1,1-dimethylethyl]adimethylethyl]adimethylethyl]adimethylethyl]adimethylethyl]adimethylethyl]-3,3'-dimethylethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidenejmethyl]-3,3'-dimethyl[2,2'-bithiophen]-5-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

(Continued)

L65 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Cor RN 402857-28-7 CAPLUS CN Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5'-[[6-[(1E)-2-[4-

(dibutylamino)phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

PAGE 1-A

PAGE 1-B

402857-26-5P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(nonlinear optical devices employing second-order nonlinear optical
chromophores containing dioxin and/or bithiophene as conjugate bridge)
402857-26-5 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5'-[[6-[(1E)-2-[4-[bis[2-[[(1,1dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2,2-dimethyl4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihayl[2,2'-bithiophen]-5yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

L65 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2002:172353 Document No. 136:2388020 Second-order nonlinear optical
chromophores containing dioxin and/or bithiophene as conjugate bridge and
devices incorporating the same. Wang, Chuanguang; Zhang, Cheng;
Fetterman, Barold R.; Steler, William; Michael, Joseph (Pacific Wave
Industries, Inc., USA). U.S. Pat. Appl. Publ. US 2002007220 Al
20020307, 16 pp., Cont.-in-part of U. S. Ser. No. 488,422.
(English). CODEN: USXXCO. APPLICATION: US 2001-998625 20010703.
PRICRITY: US 2000-488422 20000120; US 1998-122806 19980727; US
2000-546930 20000411; US 2000-551685 20000418.

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Nonlinear optical devices (e.g., electrooptical modulators, phase shifters) comprising an active element formed from a chromophore including an electron donor group, an electron acceptor group, and a bridge structure between the electron donor group and the electron acceptor

group

are described in which the chromophores is described by the general formula I, the bridge structure is described by the general formula II,

the electron donor group and the bridge structure are described by the general formula III (A = CHZ or O; B = is an electron acceptor; and R = independently selected H, F, or a perhalogenated, halogenated, or nonhalogenated Cl-30 aliphatic or aromatic group functionalized with ≥0 hydroxy, ether, ester, amino, silyl, and siloxy groups).

402857-28-7

RL: DEV (Device component use); USES (Uses)

(nonlinear optical devices employing second-order nonlinear optical chromophores containing dioxin and/or bithiophene as conjugate bridge)
402857-27-6 CAPLUS

Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5'-[(1E)-2-[4-

(diethylamino)phenyl]ethenyl]-3,3'-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

GT

L65 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

ANSWER 27 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2:142698 Document No. 136:2239410 Design and synthesis of advanced NLO
materials for electro-optic applications. Londergan, Tim; Todorova,
Galina K., Zhu, Jingsong; Huang, Diyun (Lumera Corporation, USA). PCT
Int. Appl. WO 2002014305 A2 20020221, 119 pp. DESIGNATED
STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BB, GB, BR, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, II, IN, IS, JP, KR, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MM, MM, MK, MZ, NO, NZ, PH, PL, FT, RO, RU, SD, SE,
SG, SI, SK, SL, TU, TM, TR, TI, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM; RN: AT, BE, BF, BJ, CF, CG, CH, CI, CM,
CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, MI, MR, NE, NL, PT,
SE, SN, TD, TG, TR. (English). CODEN: PIXXD2 APPLICATION WO
2001-US25779 20010817. PRIORITY: US 2000-226267P 20000817.

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Thiophene-containing chromophores are described by the general formulas I, II

I and III (D = electron donating group with low electron affinity relative to the electron affinity of  $\lambda$ ;  $\pi 1, 2$  are absent or a bridge that provides electronic conjugation between the thiophene ring and D or  $\lambda$ , resp.;  $\lambda$  = electron accepting group with high electron affinity relative to the electron affinity of D; X = O or S;  $\lambda$  = alkyl, aryl, heteroalkyl

heteroaryl; n = 1-4; R1,2 = alkyl, aryl or heteroalkyl;  $\pi$  is absent or a bridge that provides electronic conjugation between D1 and the double bond adjacent to  $\pi$ ; D1 = is an electron donating group with low electron affinity relative to the electron affinity of the fragment to which  $\pi$  is connected). Also described are processes for providing materials comprising the novel chromophores and polymer matrixes sixten containing

the novel chromophores. Electrooptical devices containing one or more of the

described electron acceptors, electron donors, conjugated bridges, or chromophores are also discussed. 400760-64-7P 400760-71-6P 400771-39-3P RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (design and synthesis of advanced nonlinear optical materials for

(design and synthesis of advanced nonlinear optical materials for electrooptical applications) 400760-64-7~CAPLUS Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[3,4-dibutoxy-5-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 2-A

L65 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

400760-71-6 CAPLUS Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-8]-2-1]-4-1]-4-1])

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutoxy-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

400771-39-3 CAPLUS
Propanedinitrile, [3-cyano-4-[(1E)-2-[[[[(1,1-dinethylethyl)dimethylsily1]oxy]methyl]-7-[(1E)-2-[4-[ethyl(2-hydroxyethyl)dimino]phenyl]ethenyl]-2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yllethenyl]-5,3-dimethyl-2(5H)-furanylidene]-(9CI) (CA INDEX NAME)

L65 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2002:136097 Document No. 136:1914420 Sterically stabilized polyene-bridged
second-order nonlinear optical chromophores and devices incorporating the
same. Zhang, Cheng; Fetterman, Harold R.; Steier, William; Michael,
Joseph (Pacific Wave Industries, Inc., USA). U.S. US 6346992 B1
20020219, 33 pp., Cont.-in-part of U.S. Ser. No. 546,930.
(English). CCDEN: USXXAM. APPLICATION: US 2000-51685 20000418.
PRIORITY: US 1999-122806 19980727; US 2000-488422 20000120; US
2000-546930
20000411.
AB Nonlinear optical devices (e.g., electrooptical modulators, phase
shifters) are described which employ an active element formed from a
chromophore including an electron donor group, an electron acceptor
group,

group,
and a π-conjugate bridge structure between the electron donor group and
the electron acceptor group which includes ≥1 non-aromatic 5-, 6-, or
7-membered ring which lock(s) one or two carbon-carbon double bond(s) of
the conjugate bridge structure and in which the electron acceptor group

connected to the bridge ring structure with a conjugated diene or triene. The bridge may contain a bithiophene unit. The chromophores may be doped into a polymer, preferably a bisphenol A carbonate-4,4'-(3,3,5-trimethyleyclohexylidene)diphenol carbonate copolymer. The devices may be packaged in inert gas filled packages. 369397-36-4P

369397-36-4P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(nonlinear optical devices employing sterically stabilized
polyene-bridged second-order nonlinear optical chromophores)
3397-36-4 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5'-[[3-[2-[4-

(dimethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]methyl]3,3'-dihexyl[2,2'-bithlophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]- (CA INDEX NAME)

PAGE 1-A Me- (CH2) 5 (CH<sub>2</sub>)<sub>5</sub>-Me

PAGE 1-B

ANSMER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2:90034 Document No. 136:1362450 Hyperpolarizable organic chromophores.
Dalton, Larry R.; Jen, Alex Kwan-Yue; Londergan, Timothy; Carlson,

Brenden; Phelan, Gregory; Huang, Diyun; Casmier, Daniel; Ewy, Todd;

Buker, Nicholas (University of Washington, USA). PCT Int. Appl. WO 2002008215

Nicholas (University of Washington, USA). PCT Int. Appl. WO 2002008215
20020131, 104 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU,
AZ, BA, BB, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ,
EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG,
KF, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ,
NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
UG, US, UZ, VM, VU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, EM+ AT,
BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE,
IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN:
PIXXD2. APPLICATION: WO 2001-US23339 20010724. PRIORITY: US
2000-EV220321 20000724.
The present invention provides hyperpolarizable organic chromophores
ed on
heterocyclic compds. The chromophores are nonlinear optically active
compds. that include a π-donor conjugated to a π-acceptor through a
π-electron conjugated bridge. Macromol, structures including the
hyperpolarizable organic chromophores are also provided.
392662-44-IP 392662-45-2P;
RL: IMF (Industrial manufacture); TEM (Technical or engineered material
use); PERF (Preparation); USES (Uses)
(chromophore; production of donor-acceptor conjugated hyperpolarizable
heterocyclic organic chromophores)
392662-44-1 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[7-((1E)-2-[4-[bis(4hoxyphenyl] amino] bhenyl]-2,3-dihydrothieno(3,4-b)-1,4-dioxin-5-

methoxyphenyl)amino]phenyl]ethenyl]-2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl]ethenyl]-3-cyanodihydro-5,5-dimethyl-2(3H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

392662-55-4P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (dendriner chromophore; production of donor-acceptor conjugated hyperpolarizable heterocyclic organic chromophores)
392662-55-4 CAPLUS
Benzoic acid, 3,5-bis(phenylmethoxy)-,

[[4-[(1E)-2-[4-[[[3,5-bis(phenylmethoxy)benzoyl]oxy]methyl]-5-[(1E)-2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

392662-45-2 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis (4-methoxyphenyl)amino]phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-3-cyanodihydro-5,5-dimethyl-2(3H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

392662-59-8P 392662-63-4P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(green chromophore; production of donor-acceptor conjugated hyperpolarizable heterocyclic organic chromophores)
32662-59-8 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[(1E)-2-[5-[(1E)-2-[4-

(diethylamino)phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

 $\rm L65$  ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN Double bond geometry as shown. (Continued)

392662-63-4 CAPLUS
Propanedinitrile, 2=[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-[[(1,1-dimethylathyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]thieno[3,2-b]thien-2-yl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA) INDEX

NAME)

Double bond geometry as shown.

PAGE 1-B

392662-54-3

L65 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002:49603 Document No. 136:332344 Highly efficient and thermally stable organic/polymeric electro-optic materials by dendritic approach. Jen, Alex K.-Y.; Ma, Hong; Sassa, Takafumi; Liu, Sen; Suresh, S.; Dalton,

Alex K.-Y., Ma, Hong; Sassa, Takafumi; Liu, Sen; Duresn, D.; Dallon,
Larry
Raymond; Haller, Marnie (Department of Materials Science and Engineering,
University of Washington, Seattle, WA, 98195-2120, USA). Proceedings of
SPIE-The International Society for Optical Engineering, 4461(Linear and
Nonlinear Optics of Organic Materials), 172-179 (English) 2001.
CODEN: PSISDO. ISSN: 0277-786X. Publisher: SPIE-The International
Society for Optical Engineering.

AB Dendron-modified nonlinear optical (NLO) chromophores and multiple
chromophore-containing crosslinkable NLO dendrimers were developed. The
enhancement of poling efficiency (40%) in the dendritic NLO
chromophore/polymer guest/host system was obtained due to the significant
minimization of internol. electrostatic interactions among chromophores
by

the dendritic effect. Multiple NLO chromophore building blocks can be further placed into a dendrimer to construct precise mol. architecture with predetd. chemical composition The site-isolation effect, through

the
encapsulation of NLO moieties by dendrons, can greatly enhance the
performance of electrooptic (E-O) materials. A very large E-O
coefficient (r33
= 60 pm/V at 1.55 µm ) and high temporal stability (85° C for
>1000 h) were achieved in a NLO dendrimer developed through the

double-end

>1000 h) were achieved in a NLO dendrimer developed through the let-end functionalization of a 3-dimensional shape phenyl-tetracyanobutadienyl (Ph-TCBD) - containing NLO chromophore with thermally crosslinkable trifluorovinylether-containing dendrons.
413627-45-9 413627-50-6 413627-55-1 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (highly efficient and thermally stable organic/polymeric electro-optic materials by dendritic approach)
413627-45-9 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5-[4-[4-(dibutylamino)phenyl]-1,3-butadien-1-yl]-4-[[([1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thienyl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

413627-50-6 CAPLUS
Tricyclo[3.3.1.13,7]decane-1-carboxylic acid,
[5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3-furanyl]efthenyl]-2-[4-[4-(dibtylamino)phenyl]-1,3-butadien-1-yl]-3-thienyl]methyl ester (CA INDEX NAME)

L65 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prodn. of donor-acceptor conjugated hyperpolarizable heterocyclic org. chromophores)
RN 392662-54-3 CAPLUS
CN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3-(hydroxymethyl)-2-thienyl]ethenyl]-5,5-dibutyl-3-cyano-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

413627-55-1 CAPLUS

Benzoic acid, 3,5-bis[(2-ethylhexyl)oxy]-,
[5-[2-[4-cyano-5-(dicyanomethylene)-2,5-dihydro-2,2-dimethyl-3furanyl]lethenyl]-2-[4-[4-(dibtylamino)phenyl]-1,3-butadien-1-yl]-3thienyl]methyl ester (CA INDEX NAME)

L65 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) L65 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

CH2

(Continued) PAGE 3-A

PAGE 1-A

PAGE 2-A

L65 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2001:935613 Document No. 136:552260 Chromophores, their production and

r
use for polymeric thin films and optical waveguides. He, Mingqian;
Lesle, Thomas M. (Corning Incorporated, USA). FCT Int. Appl. WO
2001098310 Al 20011227, 48 pp. DESIGNATED STATES: W: AE, AG,
AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BY, BZ, CA, CH, CN, CR, CU, CZ, DE,
DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP,
KE, KG, KP, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM,
MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
TZ, UA, UG, UZ, VN, YU, ZA, ZW; RW: AT, BE, CH, CY, DE, DK, ES, FI, FF,
GB, GR, IE, IT, LU, MN, NL, PT, SE, TR. (English). CODEN: PIXND2.
APPLICATION: WO 2001-US15827 20010516. PRIORITY: US 2000-595221
0616;

APPLICATION: wo Low ...
20000616;
US 2000-675966 20000929.

AB The present invention is directed to chromophores having novel electron-withdrawing groups and novel bivalent cyclic bridges and to optical waveguides and optical devices having polymeric thin films which contain the novel chromophores. An example was given for the production of

containing introduced introduced to a conjugated containing thiophene and dihydrofuran rings; this compound was copolymd. with a chlorinated norbornenedicarboxylic acid derivative and a chlorinated xylylenediol to provide an electrooptical polyester.

IT 383124-85-4P

Journal of Temperature (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREF (Preparation); RACT (Reactant or reagent); USES (Uses)

(monomer chromophore; production of intermediates for electrooptical

monomer chromophore; production of intermediates for electrooptical
chromophores)
383124-85-4 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

383124-86-59
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(monomeric chromophore; production of intermediates for electrooptical

L65 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2002:17434 Document No. 137:7001 Compact EO polymer vibration sensors utilizing various planar and hybrid fiber/waveguide architectures. Yacoubian, Araz (IPITEK, Carlsb

Yacoubian, Araz (IPITEK, Carlsbad, CA, 92008, USA). Polymer News, 2), 408-415 (English) 2001. CODEN: FLYNBU. ISSN: 0032-3918. Publisher: Gordon & Breach Science Publishers.

The use of electro-optic (EO) polymers for high frequency vibration sensing applications is explored. This paper presents four integrated optics-based sensor architectures designed to perform acoustic spectrum anal. These devices utilize EO polymer materials traditionally used for communication applications, whereas here they are used to perform heterodyning to down-convert high frequency (GHz) vibrations to lower frequencies and utilize low-frequency photo detectors. In conjunction with a pulsed laser, the sensors are capable of interrogating sub-surface structures of thin films and opaque materials at micron and sub-micron depth resolution. To make a practical device requires addressing loss, size,

mech. and thermal fluctuation tolerance, and ease of fabrication issues. Therefore, four different architectures are implemented and compared.

implemented devices consist of planar wavequide and fiber structures utilizing ridge, slab mode, hybrid ridge/slab mode, and hybrid fiber/waveguide architectures. Performances of all four devices are compared, and the best architecture is chosen. Low-frequency expts. Illustrate the proof of concept, while high frequency expts. (measure to 200 MHz) illustrate the sensing of vibration excited by a pulsed MG Low-frequency expts. Nd-YAG

laser. Application of the technol, for different industries is

discussed. IT 432555-91-4

IT 432555-91-4

RI: DEV (Device component use); PRP (Properties); USES (Uses)

(compact electro optic polymer vibration sensors utilizing various planar and hybrid fiber/waveguide architectures)

RN 432555-91-4 CAPLUS

CN Propanedinitrile,

[4-[2-[5-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-,

homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 224746-62-7 CMF C36 H42 N4 O3 S

L65 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

chromophores) 383124-86-5 CAPLUS

Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

383124-87-6P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (USES)
(production of polyesters containing electrooptical chromophores)
383124-87-6 CAPLUS
Bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl dichloride,
1,4,5,6,7,7-hexachloro-, polymer with

[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-4-decyl-2-thienyl]ethenyl]-3-cyano-5-(3,4-dichlorophenyl)-5-methyl-2(5H)-furanylidene]propanedinitrile and 2,3,5,6-tetrachloro-1,4-benzenedimethanol (9CI) (CA INDEX NAME)

CM 1

CRN 383124-85-4 CMF C43 H46 C12 N4 O3 S

Double bond geometry as shown.

L65 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

3 CM

CRN 7154-26-9 C8 H6 C14 O2

L65 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2001:781221 Document No. 135:3367150 Sterically stabilized polyene-bridged second-order nonlinear optical chromophores and devices incorporating the same. Zhang, Cheng; Fetterman, Harold R.; Steier, William; Michael, Joseph (Pacific Wave Industries, Inc., USA). FCT Int. Appl. WO
201079750 A1 20011025, 64 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DM, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, UJ, DJ, IN, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NO, NZ, PL, PT, RO, RU, SD, S, SG, SI, SS, LT, TM, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, KN: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, RG, IE, IT, LU, APPLICATION: WO 2001-US1254 20010416. PRIORITY: US 2000-551685
20000418.

AB Nonlinear optical devices (e.g., electrooptical modulators, phase shifters) are described which employ an active element formed from a chromophore including an electron donor group, an electron acceptor group,

group,

 $^{2}$ , and a π-conjugate bridge structure between the electron donor group and the electron acceptor group which includes ≥1 non-aromatic 5-, 6-, or 7-membered ring which lock(s) one or two carbon-carbon double bond(s) of the conjugate bridge structure and in which the electron acceptor group

connected to the bridge ring structure with a conjugated diene or triene. The bridge may contain a bithiophene unit. The chromophores may be doped into a polymer, preferably a bisphenol A carbonate-4,4'-(3,3,5-trimethylcyclohexylidene)diphenol carbonate copolymer. The devices may be packaged in inert gas filled packages. 369397-36-49P

36939/-36-4F RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(Reactant or reagent)
(nonlinear optical devices employing sterically stabilized polyene-bridged second-order nonlinear optical chromophores)
369397-36-4 (APLUS

369397-36-4 CAPLUS
Propanedinitrile, 2-[3-cyano-4-[2-[5'-[[3-[2-[4-

(dimethylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]methyl]3,3'-dihexyl[2,2'-bithlophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)furanylidene]- (CA INDEX NAME)

PAGE 1-A

L65 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B

- NMe2

L65 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2001:545954 Document No. 135:1444920 Sterically stabilized second-order nonlinear optical chromophores and devices incorporating the same.
Dalton, Larry R; Zhang, Cheng, Wang, Chuanguang; Fetterman, Harold R;
Wang, Fang; Steier, William; Harper, Aaron W.; Ren, Albert S.; Michael,
Joseph (Pacific Wave Industries, Inc., USA). PCT Int. Appl. WO
2001053746

D53746
A1 20010726, 52 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, EY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, RP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NO, NZ, PL, FT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UJ, UG, US, UZ, VM, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW, AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, FT, SE, SN, TD, TG, TR. (Equish). CODEN: PIXXD2. APPLICATION: WO 2001-US1655 20010117. PRIORITY: US 2000-488422

PIXXD2. APPLICATION: WO 2001-US1655 20010117. PRIORITY: US 2000-488422 20000120.

Nonlinear optical devices are described in which the active element incorporates a chromophore which includes an electron donor group and an electron acceptor group joined by a bridge structure, preferably a ring-locked bridge structure. Preferably, at least the electron acceptor group is bonded to the bridge structure via a conjugated diene. In a preferred embodiment, the bridge structure also includes at least one bulky side group. The bridge structure may comprise two protected alicyclic rings or ring-locked trienone. Alternately, the chromophore

include an electron donor group, a ring-locked tricyano electron acceptor group, and a bridge structure between them. The electron acceptor group may comprises an isophorone structure. The bridge structure may include

bithiophene unit or a a modified isophorone unit. 351445-08-4 351445-10-8 RL: DEV (Device component use); USES (Uses) (nonlinear optical devices employing sterically stabilized

(nonlinear optical devices employing sterically stabilized second-order nonlinear optical chromophores)

RN 351445-08-4 CAPLUS
CN Propanedinitrile,
2-[3-cyano-4-[2-[5'-[2-[4-(diethylamino)phenyl]ethenyl]-3,3''-dihexyl[2,2'-bithiophen]-5-yl]ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

351445-10-8 CAPLUS Propanedinitrile, 2-[4-[5'-[[6-[2-[4-[bis[2-[[(1,1-

L65 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) dimethylethylldimethylsiylloxyjethyllaminojphenyllethenyll-2,2-dimethyl-4H-1,3-dioxin-4-ylidenelpmethyll-3,7-diohexyl[2,2'-bithiophen]-5-yllethenyll-3-cyano-5,5-dimethyl-2(5H)-furanylidenel- (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

L65 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2001:544550 Document No. 135:2886460 Rapid and efficient synthesis of 2-[3-cyano-4-(2-arylidene)-5,5-dimethyl-5H-furan-2-ylidene)-malonon under focused microwave irradiation. Villemin, Didier; Liao, Liang

under focused microwave irradiation. Villemin, Didier; Liao, Liang le
Nationale Superieure d'Ingenieurs de Caen, ISMRA, UNR CNRS 6507, Caen,
F-14050, Fr.). Synthetic Communications, 31(11), 1771-1780 (English)
2001. CODEN: SYNCAV. ISSN: 0039-7911. OTHER SOURCES: CASREACT
135:288646. Publisher: Marcel Dekker, Inc..
New biol. potential (2-furanylidene)malonitriles were synthesize
efficiently by one-pot condensation under focused microwave from starting
and easy available compds. An example compound thus prepared was
[3-cyano-4+[(E)-2-(2-furanyl)+thenyl]-5,5-dimethyl-2(5H)furanylidene)propanedinitrile.
364599-38-0.P 364599-37-1P 364599-38-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [3-cyano-4+[(E)-2-(aryl)+thenyl]-5,5-dimethyl-2(5H)furanylidene)propanedinitriles)
36599-36-0 CAPLUS
Propanedinitrile, 2-[3-cyano-4+[(E)-2-(2-furanyl)+thenyl]-5,5-dimethyl2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

364599-37-1 CAPLUS
Propanedinitrile, 2-[3-cyano-5,5-dimethyl-4-[(1E)-2-(2-thienyl)ethenyl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

364599-38-2 CAPLUS Proparedinitrile, 2-(3-cyano-5,5-dimethyl-4-[(1E)-2-(3-thienyl)ethenyl]-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSWER 36 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN :425192 Document No. 135:218335 Production of high bandwidth polymeric electro-optic modulators with Vx voltages of less than 1 volt. Dalton, Larry; Robinson, Bruce; Steier, William (Department of Chemistry, University of Washington, Seattle, WA, 98195-1700, USA). MCLC S67, Section B: Nonlinear Optics, 25(1-4), 23-34 (English) 2000. CODEN: MCLCB. ISSN: 1058-7268. Publisher: Gordon & Breach Science Publishers.

CODEN: MLICOR. 1858. 1857. Publishers.
Structure/function relations crucial to realization of broad bandwidth, low halfwave voltage, high stability polymeric electrooptic modulators

discussed. Particular attention is given a family of chromophores

discussed. Particular attention is given a family of chromophores containing cyanofuran acceptors. Such chromophores permit the simultaneous realization of large mol. hyperpolarizability and thermal stability. The role of intermol. electrostatic interactions in limiting maximum achievable macroscopic electrooptic activity is discussed within the frameworks of both equilibrium and Monte Carlo statistical mech. calons. The processing of polymeric electrooptic materials into low optical loss, 3-dimensional optical circuits is discussed. Finally, the use of polymeric electrooptic circuits for realization of phased array radar, time stretching, and other

device applications is reviewed. 213313-98-7 265932-54-9 RL: DEV (Device component use); MCA (Modifier or additive use); USES (Uses)

(production of high bandwidth polymeric electro-optic modulators with

voltages of less than 1 V)
213131-98-7 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

265992-54-9 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2(acetyloxy)ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2000:876115 Document No. 134:179119 Progress toward Device-Quality
Second-Order Nonlinear Optical Materials. 4. A Trilink High µB NLO
Chromophore in Thermoset Polyurethane: A "Guest-Host" Approach to Larger
Electrooptic Coefficients. Zhang, Cheng; Wang, Chuanguang; Dalton, Larry
R.; Zhang, Bua; Steier, William H. (Loker Hydrocarbon Institute and
Department of Chemistry, University of Southern California, Los Angeles,
CA, 90089-1661, USA). Macromolecules, 34(2), 253-261 (English)
2001. CODEN: MAMOREX. ISSN: 0024-9297. Publisher: American
Chemical Society.

AB A tri-linkable thiophene-containing second-order nonlinear optical (NLO)
chromophore [(HO)3FTC] was synthesized from a tri-linkable donor bridge
and a tri-cyanofuran electron acceptor (TCF). The TCF acceptor was
modified with two Bu groups which greatly increased solubility and
processability of the tribydroxy-functionalized chromophore and inhibited
strong Chromophore-chromophore interaction. A thermal stability study of
(HO)3FTC indicates that the free hydroxyl group located close to the
Cyano cyano

acceptor causes the chromophore to decompose at a much lower temperature than  $\ensuremath{\operatorname{FTC}}$ 

chromophores with no free hydroxyl groups. Significantly improved

thermal

mal stability of the chromophore in a polyurethane film was obtained by masking the free hydroxyl groups with toluene diisocyanate (TDI). Folyurethane prepolymer synthetic schemes were designed and studied in detail to improve elec. field induced dipole alignment. Enhancement of over 150% in poling efficiency was achieved by reducing the degree of chromophore attachment to the polymer backbone before applying an elec. poling field through a guest-host approach. It was critical to allow TDI and

triethanolamine hydroxyl cross-linkers to react at higher temperature for a

longer time to form a partially cross-linked prepolymer before the -NCO masked trillink chromophores to a three-dimensional cross-linked polyurethane network at three points, the thermal stability of poling-induced electrooptic activity was enhanced by

268548-55-6P

L65 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued) Aco-CH2-CH2

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

326597-51-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (monomer, trifunctionalized chromophore; preparation of trifuncyanate-thiophene chromophore and incorporation to TDI-TEA prepolymer to obtain polyurethane second-order NLO with high poling

prepolymer to obtain polyuretname actions of the control of the efficiency)
326597-51-7 CAPLUS
Carbamic acid, (3-isocyanato-4-methylphenyl)-,
[[4-[2-[5-[2-2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-4-[[[[(3-isocyanato-4-

methylphenyl)amino]carbonyl]oxy]methyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-A

IT 326597-52-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polyurethane; preparation of triisocyanate-thiophene chromophore and incorporation to TDI-TEA prepolymer to obtain polyurethane second-order
NLO with high poling efficiency)
RN 326597-52-8 CAPLUS
CN Carbamic acid, (3-isocyanato-4-methylphenyl)-,
[[4-[2-[5-[2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-4-[[[[3-isocyanato-4-

methylphenyl)amino]carbonyl]oxy]methyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester, polymer with 2,4-diisocyanato-1-methylbenzene and

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

PAGE 2-A

CM 2 CRN 584-84-9 CMF C9 H6 N2 O2

см з

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2,2'.-nitrilotris[ethanol] (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 326597-51-7 CMF C62 H58 N10 O10 S

L65 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 102-71-6 CMF C6 H15 N O3

сн2-сн2-он но-сн<sub>2</sub>-сн<sub>2</sub>-и-сн<sub>2</sub>-сн<sub>2</sub>-он

ANSWER 38 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
1819787 Document No. 134:123327 Realization of polymeric electro-optic modulators with less than one volt drive voltage requirement. Zhang, Cheng; Lee, Michael; Winklemann, Adam; Northeroft, Beidi; Lindsey, Christopher; Jen, Alex K. Y.; Londergan, Timothy; Steier, William H.; Balton, Larry R. (Loker Hydrocarbon Research Institute, University of Southern California, Los Angeles, CA, 90089-1661, USA). Materials Research Society Symposium Proceedings, 590 (Electrical, Optical, and Magnetic Properties of Organic Solid-State Materials VI, BB4.2/1-BB4.2/12 (English) 2000. CODEN: MRSPDH. ISSN: 0272-9172. Publisher:
Materials Research Society.
The roles played by spatially anisotropic intermol. electrostatic interactions, chromophore shape, host dielec. constant, and poling field strength in defining maximum achievable electrooptic activity for elec.

chromophore/polymer materials were studied by equilibrium and Monte-Carlo quantum statistical mech. calons. Even simple Hamiltonians reproduce critical qual. features such as the existence of a maximum in plots of electrooptic activity vs. chromophore number d. in a polymer matrix. Comparison of theor. results for various methods provides a useful check on the validity of approxns. employed with individual methods. The most significant conclusion to derive from a comparison of exptl. and theor. results is the dependence of maximum achievable electrooptic activity

chromophore shape. Theor. calcns. suggest a new paradigm for the design of optimum electrooptic chromophores; realization of the desired shapes may be facilitated by dendritic synthetic approaches. In the presence of intermol. electrostatic interactions, the dependence of electrooptic activity upon material dielec. permittivity and elec. poling field strength is more complex than in the absence of such interactions. Of particularly, interest are conditions that lead to 2nd order phase transitions to lattices containing centrically (antiferroelectrically) ordered chromophore domains. Such phase transitions can lead to further complications in the attempted preparation of device quality materials can

be effectively avoided using theor. derived phase diagrams.

(Physical, engineering or chemical process); PRP (Properties);

(realization of polymeric electro-optic modulators with less than one drive voltage requirement) 47-0 CAPLUS

321164-47-0

321164-47-0 CAPUS
Benzoic acid, 3,5-bis(phenylmethoxy)-,
[[4-[2-[5-[2-[2-[4-[[3,5-bis(phenylmethoxy)benzoyl]oxy]butyl]-4-cyano-5(dicyanomethylene)-2,5-dihydro-2-methyl-3-furanyl]ethenyl]-3,4-dibutyl-2thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI) (CA INDEX

L65 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued)

PAGE 1-B — ph

L65 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
2000:336442 Document No. 133:24424 Optical intensity modulator based on a novel electrooptic polymer incorporating a high μβ chromophore.

Lee, Sang-Shin, Carner, Sean M.; Chuyanov, Vadim; Zhang, Hua; Steier, William H.; Wang, Fang; Dalton, Larry R.; Udupa, Anand H.; Fetterman, Harold R. (Department of Electrical Engineering-Electrophysics, University of Southern California, Los Angeles, CA, 90099-0483, USA). IEEE Journal of Quantum Electronics, 36(5), 527-532 (English) 2000. CODEN: IEJOA7. ISSN 018-9197. Publisher: Institute of Electrical and Electronics Engineers.

AB The authors synthesized a novel electrooptic (EO) polymer based on a high μβ chromophore incorporating tricyanobutadiene acceptors. A crosslinked polyurethane network was also adopted to enhance its thermal stability. To find the optimum poling condition for the polymer, the influence of the elec. poling profile on optical characteristics such as EO effect, thermal stability, and damage was studied. Then a high-speed intensity modulator using the EO polymer was designed and fabricated.

measured half-wave voltage  $V\pi$  was 4.5 V at the wavelength of 1.31  $\mu m$ . Accordingly, the achieved EO coefficient r33 was  $\leq$ 25 pm/V, and the thermal stability of the poled polymer was  $\leq$ 95°. Finally, the modulator was successfully operated up to 40 GHz. 247088-15-9P

247088-15-9P RLi DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (optical intensity modulator based on novel electrooptic polymer incorporating high  $\mu\beta$  chromophore) 247088-15-9 CAPLUS

Propanedinitrile, [4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethy1)amino]pheny1]etheny1]-3,4-dibuty1-2-thieny1]etheny1]-3-cyano-5,5-dimethy1-2(5H)-furanylidene]-, polymer with 1,3-diisocyanatomethylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 247088-12-6 CMF C36 H42 N4 O3 S

Double bond geometry as shown.

L65 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

D1-Me

ANSWER 40 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1:248019 Document No. 122:340819 Monte Carlo statistical mechanical simulations of the competition of intermolecular electrostatic and poling-field interactions in defining macroscopic electro-optic activity for organic chromophore/polymer materials. Robinson, B. H.; Dalton, L. 2000:248019

(Department of Chemistry, University of Washington, Seattle, WA, 98195-1700, USA). Journal of Physical Chemistry A, 104(20), 4785-4795 (English) 2000. CODEN: JFCAFH. ISSN: 1089-5639. Publisher: American Chemical Society. Wonte Carlo statistical mech. computer simulations of the elec.-field poling of 2nd-order nonlinear optical chromophores, characterized by

dipole moments, polarizabilities, and hyperpolarizabilities, are presented. Such theor. anal. is critical to defining the structure/function relationships that permit maximization of electrooptical activity for melectron chromophore-containing polymeric materials. Polymeric electrooptical materials may, in turn, be important for high-bandwidth telecommunications, new forms of radar, and high-speed data processing. The exptl. observed maxima in plots of electrooptical activity vs. chromophore number d. (loading) in polymer matrixes are theor. reproduced, as are the shifts of the maxima to lower loading with increasing chromophore dipole moment. Modification of the chromophore shape to realize the maximum

maximum achievable electrooptical activity for a given  $\pi$ -electron structure is discussed, as is the role of polymer elec. permittivity. Monte Carlo results are compared with the results of equilibrium statistical mech.

based on the approximation of Piekara. The theor. results presented

led to the production of polymeric electrooptical materials that permit devices with drive voltage requirements of <1 V to be fabricated. Polymeric modulators now significantly exceed the performance capabilities

oilities
(in terms of bandwidth and drive voltage) of electrooptical modulators
based on inorg. materials.
267664-48-2D, amino and thienyl derivs.
RL: MOA (Modifier or additive use); PEP (Physical, engineering or

IT

chemical

process); FRP (Properties); PROC (Process); USES (Uses)
 (dopant; Monte Carlo statistical mech. simulations of the competition
 of intermol. electrostatic and poling-field interactions in defining
 macroscopic electrooptical activity for organic chromophore/polymer
 materials)

RN 267664-48-2 CAPLUS

CN Propanedinitrile,
2-[4-[2-[5-[2-4-aminophenyl)ethenyl]-2-thienyl]ethenyl]3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2000;245052 Document No. 132:315554 Low (sub-1-volt) halfwave voltage polymeric electro-optic modulators achieved by controlling chromophor shape. Shi, Yongqiang; Zhang, Cheng; Zhang, Hua; Bechtel, James H.; Dalton, Larry R.; Robinson, Bruce H.; Steier, William H. (TACAN Corporation, Carlsbad, CA, 92008, USA). Science (Washington, D. C.), 288(5463), 119-122 (English) 2000. CODEN: SCIENS. ISSN. 0036-8075. Publisher: American Association for the Advancement of Science.

0U30-8U/5. Publisher: American Association for the Advancement or Science. Science. Electrooptic (EO) modulators encode elec. signals onto fiber optic transmissions. High drive voltages limit gain and noise levels. Typical polymeric and Li niobate modulators operate with halfwave voltages of 5

Sterically modified organic chromophores were used to reduce the

attenuation of elec. field poling-induced electrooptic activity caused by strong intermol. electrostatic interactions. Such modified chromophores, incorporated into polymer hosts, were used to fabricate EO modulators

halfwave voltages of 0.8 V (at a telecommunications wavelength of 1318

and to achieve a halfwave voltage-interaction length product of 2.2 Vand to achieve a halfwave voltage-interaction length product of 2.2 V-centimeters. Optical push-pull poling and driving were also used to reduce halfwave voltage. This study, together with recent demonstrations of exceptional bandwidths (more than 110 GHz) and ease of integration (with very large scale integration semiconductor circuitry and ultra-low-loss passive optical circuitry) demonstrates the potential of polymeric materials for next generation telecommunications, information processing, and radio frequency distribution. 213131-98-7 265992-54-9

233313-98-7 265992-54-9
RL: PRP (Properties)
(low (sub-1-V) halfwave voltage polymeric electro-optic modulators achieved by controlling chromophore shape)
213131-98-7 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis [2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

265992-54-9 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-(acetyloxy)ethyl]maino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1:208420 Document No. 132:335227 Dendrimer functionalized NLO chromophores. Londergan, Timothy M.; Zhang, Cheng; Ren, Albert; Dalton, Larry (Department of Chemistry, University of Washington, Seattle, WA, 98195, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 41(1), 783-784 (English) 2000. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry. Polymer Chemistry), 41(1), 78-764 [English 2000. CODEN:
ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB We have synthesized a Ph benzyl ether dendrimer containing an FTC chromophore
in the core. This serves to isolate the nonlinear optical (NLO) active FTC mol. from neighboring chromophores, thereby decreasing the intermedic electrostatic interactions. The structure of the FTC-dendrimer was confirmed by 1H NNMR, 13C NNMR, and MALDI-TOF mass spectrometry.

IZ 269548-55-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of dendrimer-functionalized furanyl-thienyl-cyano-containing nonlinear optical chromophores)

RN 269548-55-6 CAPLUS
CN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3-(hydroxymethyl)-2-thienyl]ethenyl]-5,5-dibutyl-3-cyano-2(5H)-furanylidene]- (CA INDEX NAME)

IT

208348-5/-8F Rf. SPN (Synthetic preparation); PREP (Preparation) (preparation and characterization of) 268548-57-8 CAPLUS Benzoic acid, 3,5-bis(phenylmethoxy)-,

[[4-[2-[4-[[[3,5-bis(phenylmethoxy)benzoyl]oxy]methyl]-5-[2-[2,2-dibutyl-4-cyano-5-(dicyanomethylene)-2,5-dihydro-3-furanyl]ethenyl]-2-thienyl]ethenyl]phenyl]imino]di-2,1-ethanediyl ester (9CI) (CA INDEX

L65 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN

(Continued) PAGE 2-A

L65 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

L65 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2000:133769 Document No. 132:1676750 New class of high hyperpolarizability organic chromophores and process for synthesizing the same. Dalton, Larry

R1, Fetterman, Harold R1, Wang, Fang; Steier, William; Harper, Aaron W.; Ren, Albert S.; Michael, Joseph (Pacific Wave Industries, Inc., USA).

Int. Appl. Wo 2000009613 A2 20000224, 45 pp. DESIGNATED STATES:
W: AU, JP; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU,
MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US16274
1990726. PRIORITY: US 1998-122806 19980727.
The chromophores incorporate at least one organic substituent and are

formed in consideration of mol. shapes and a spatial anisotropy of intermol. interactions. The chromophores are processed into hardened material lattices to lock-in poling induced elec.-optic activity. Preferred

lattices to lock-in poling induced elec.-optic activity. Freezew organic organic substituents are alkyl, aryl, and isophorone groups. A composite including the organic chromophore, in a preferred embodiment, includes a polymer such as a poly(Me methacrylate), polyminde, polyamic acid, polystyrene, polycarbonate or polyurethane. The optimized chromophores result in hardened electro-optic polymers suitable for electro-optic modulators and other devices such as optical awitches. These modulators can be configured to work at high frequencies and in arrays for applications in communications and network connections. In addition,

they can be implemented in series and parallel combinations in phased array radar, signal processing and sensor technol. applications. 247088-14-8

RL; PRP (Properties); TEM (Technical or engineered material use); USES

(chromophores; new class of high hyperpolarizability organic chromophores

mophores
and process for synthesizing same)
247088-14-8 CAPLUS
Propanedinitrile, 2=[4=[(1E)-2-[5-[(1E)-2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

247088-13-7
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(chromophores; reaction in manufacture of new class of high hyperpolarizability organic chromophores for use in electrooptical deri

devices) 247088-13-7 CAPLUS

L65 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,-4dibutyl-2-thienyl]ethenyl]-3cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

247088-12-6P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);

(Reactant or reagent)
(intermediate; reaction in manufacture of new class of high
hyperpolarizability organic chromophores for use in electrooptical

devices)
247088-12-6 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
1999:624467 Document No. 131:350892 Theoretical investigation on the first
hyperpolarizability of push-pull polyenes containing non-aromatic cyclic
olefins. Zhu, P.; Wang, P.; Ye, C. (Institute of Chemistry, Organic
Solids Laboratory, Center for Molecular Science, Chinese Academy of
Sciences, Beijing, Peop. Rep. China). Chemical Physics Letters,
311(3.4).

Sciences, Beijing, Peop. Rep. China). Chemical Physics Letters, 311(3,4), 306-314 (English) 1999. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V.

AB Novel push-pull polyenes containing non-aromatic cyclic olefins, such as cyclopentadiene, cyclopropene and cycloheptatriene, have been investigated for application of nonlinear optical (NLO) materials. Their dot products μβ0 of first hyperpolarizability (β0) and dipole moment (μ) are calculated by employing AMI/Finite Field and ZINDO/S approaches. Among them, the largest value is as high as 4.1+10-45 esu. The origin of such high μβ0 was analyzed based on the two-level model. Non-aromatic groups can transform to a stable aromatic anion/cation through

gaining/losing an electron in their charge transfer states.

RL: PRP (Properties)

(theor. investigation on the first hyperpolarizability of push-pull polyenes containing non-aromatic cyclic olefins that become aromatic

he charge-transfer state)
213131-98-7 CAPLUS
Propanedinitrile, 2-[4-[5-[2-[4-[bis[2[acetyloxy]ethyl]amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl]-3cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 2000:24450 Document No. 132:158653 DC biased electro-optic polymer

guide
modulators with low half-wave voltage and high thermal stability. Chen,
Antao; Chuyanov, Vadim; Zhang, Hua; Garner, Sean; Lee, Sang-Shin; Steier,
William H.; Chen, Jinghong; Wang, Fang; Zhu, Jingsong; He, Mingqian; Ra,
Younsoo; Mao, Shane S. H.; Harper, Aaron W.; Dalton, Larry R.; Fetterman,
Harold R. (Department of Electrical, University of Southern California,
Los Angeles, CA, 90089-0483, USA). Optical Engineering (Bellingham,
Washington), 38(12), 2000-2008 (English) 1999. CODEN: OPEGAR.
ISSN: 0091-3286. Publisher: SPIE-The International Society for Optical
Engineering.

ISSN: 0091-3286. Publisher: SPIE-The international sourcey for operations. Engineering.

The full potential of 2nd-order nonlinear polymers can be used in electrooptic polymer modulators with a d.c. biased operation scheme to greatly reduce the half-wave voltage. This technique makes use of the total achievable electrooptic coefficient, which can be more than three

the value that was used by the conventional devices of poled electrooptic polymer. As the result of the d.c. bias and with high- $\mu\beta$  chromophores, a low half-wave voltage of 1.5 V was achieved with

2-cm-long
birefringent waveguide modulators at the wavelength of 1.3 µm. Results
of a 200° stability experiment indicate that this scheme also enables
electrooptic polymer devices to meet the short-term high-temperature

electrooptic polymer devices to meet the Short-Leam high terminal stability requirement because the polymer does not need to be poled prior to high-temperature steps.

IT 21311-98-7

RL: PRP (Properties)
(Do biased electro-optic polymer waveguide modulators with low half-wave voltage and high thermal stability)

RN 213131-98-7 CAPLUS

CN Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
1999;451775 Document No. 131:300216 Polymer electro-optic devices for
integrated optics. Steier, William H.; Chen, Antao; Lee, Sang-Shin;
Garner, Sean; Zhang, Hua; Chuyanov, Vadim; Dalton, Larry R.; Wang, Fang;
Ren, Albert S.; Zhang, Cheng; Todorova, Galina; Harper, Aaron; Fetterman
Harold R.; Chen, Datong; Udupa, Anand; Bhattacharya, Daipayan; Tsap,

(Department of Electrical Engineering, University of Southern California, Los Angeles, CA, 90089-0483, USA). Chemical Physics, 245(1-3), 487-506 (English) 1999. CODEN: CMPHC2. ISSN: 0301-0104. Publisher: Elsevier Science B.V.

A review, with 36 refs., of recent advances in electrooptic polymers and in fabrication techniques that have made possible advances in polymer optical waveguides which bring them much closer to system ready. The processing of a new thermosetting FTC polymer and its incorporation into

high-frequency, low-V $\pi$  optical amplitude modulator were reviewed. The design and fabrication of 100 GHz modulators and their integration with rectangular metal waveguides using an anti-podal finline transition with

flexible Mylar substrate was discussed. High-speed polymer modulators with balanced outputs and the in-situ trimming of the output coupler was described. More complex waveguides using polymers were demonstrated by the photonic rf phase shifter. Techniques for integrating both passive and active polymers into the same optical circuit without the need for mode matching was presented and demonstrated. To reduce the Vm of a polymer amplitude modulator to 1 V or under, a technique of constant-bias voltage was demonstrated. Finally, a technique for direct maskless laser writing in fabrication of electrooptic polymer devices was reviewed. 247088-15-9P RL: DEV (Device component use); PRP (Properties): SPN (Suntheric

247088-15-9P
RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (recent advances in electrooptic polymers in waveguides and other devices with integrated optics) 247088-15-9 CAPLUS Propanedinitrile, [4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-, polymer with 1,3-diisocyanatomethylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 247088-12-6 CMF C36 H42 N4 O3 S

Double bond geometry as shown.

L65 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

26471-62-5 C9 H6 N2 O2 IDS

D1-Me

224746-62-7, Propanedinitrile,
[4-[2-[5-[2-[4-[bis(2-hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]RI: RCT (Reactant): RACT (Reactant) or reagent)
(recent advances in electrooptic polymers in waveguides and other devices with integrated optics)
224746-62-7 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CRN 26471-62-5 CMF C9 H6 N2 O2 CCI IDS

TT 247088-14-8

24/088-14-8
RL: PRP (Properties)
(preparation and characterization of electrooptic chromophores for fabrication of electrooptic devices)
247088-14-8 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

247088-13-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of electrooptic chromophores for
fabrication of electrooptic devices)

ANSWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1:451741 Document No. 131:300096 The molecular and supramolecular engineering of polymeric electro-optic materials. Robinson, B. H.; Dalton, L. R.; Harper, A. W.; Ren, A.; Wang, F.; Zhang, C.; Todorova, G.; Lee, M.; Aniszfeld, R.; Garner, S.; Chen, A.; Steier, W. H.; Houbrecht, S.; Persoons, A.; Ledoux, I.; Zyss, J.; Jen, A. K. Y. (Department of Chemistry, University of Washington, Seattle, WA, USA). Chemical sics,

Chemistry, University of Washington, Seattle, WA, USA). Chemical Physics, 245(1-3), 35-50 (English) 1999. CODEN: CMPHC2. ISSN: 0301-0104. Publisher: Elsevier Science B.V.

AB A new class of electrooptic chromophores, of which 2-dicyanomethylen-3-cyano-4-(2-[E-(4-N,N-dl(2-acetoxyethyl)-amino)-phenylene-(3,4-dibutyl)thien-5)-E-vinyl)-5,5-dimethyl-2,5-dihydrofuran (denoted FTC) is the prototype, was prepared, characterized, and used to fabricate electrooptic devices. The mol. hyperpolarizability and thermal stability of these chromophore mols. are exceptional. Strong intermol. electrostatic interactions inhibit the efficient poling of these

mols. A statistical mech. theor. treatment is used to quant. predict the competition of poling, intermol. electrostatic interactions, and thermal effects in defining achievable acentric order and hence macroscopic optical nonlinearity. Theory is used to predict the optimum chromophore structure and material composition (chromophore loading in a polymer

structure and material composition (chromophore loading in a polymer matrix)
for maximum electrooptic activity and min. optical loss. Problems associated
with lattice hardening to lock-in poling-induced order are discussed briefly.
12 447088-15-99
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and characterization of electrooptic chromophores for fabrication of electrooptic devices)
RN 247088-15-9 CAPLUS
CN Propanedinitrile, [4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]-, polymer with 1,3-difsocyanatomethylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 247088-12-6 CMF C36 H42 N4 O3 S

Double bond geometry as shown.

L65 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 247088-13-7 CAPLUS
CN Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

IT 247088-12-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and characterization of electrooptic chromophores for fabrication of electrooptic devices)
247088-12-6 CAPLUS
Propanedinitrile, 2-[4-[(1E)-2-[5-[(1E)-2-[4-[bis(2-

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

Double bond geometry as shown.

L65 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1999:211127 Document No. 130:353208 Epoxy thermosetting NLO material.

Mingfei; Ren, Albert S.; Wang, Judy F.; Lee, Michael S.; Dalton, Larry

Zhang, Hua; Sun, Guilin; Steier, William H. (Loker Hydrocarbon Institute, University of Southern California, Los Angeles, CA, 90089, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 40(1), 162 (English) 1999. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Folymer Chemistry. A High µ-beta chromophore with epoxide functional groups was concisely synthesized by a Heck reaction. The chromophore was successfully incorporated into an epoxy thermosetting material. A 30° C increase in electro-optic thermal stability was observed as compared to

AB

hydroxyethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

224746-64-9 CAPLUS
Propanedinitrile, 2-[4-[2-[5-[2-[4-[bis(2-oxiranylmethyl)amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1999:211126 Document No. 130:352951 A trifunctionalized high  $\mu\beta$  chromophore and its 3D polyurethane network with enhanced NLO alignment stability for electro-optic device applications. Ren, Albert S.; Chen, Mingfei; Lee, Michael S.; He, Mingqian; Dalton, Larry R.; Zhang, Hua;

Guilin; Garner, Sean M.; Steier, William H. (Loker Hydrocarbon Institute, University of Southern California, Los Angeles, CA, 90089-1661, USA). Folymer Preprints (American Chemical Society, Division of Folymer Chemistry, 40(1), 160-161 (English) 1999. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.
A trifunctionalized high mu-beta chromophore, LTR, based on a dicyanomethylendihydrofuran acceptor was synthesized by coupling of a hydroxyl functionalized amino donor, a di-Bu derivatized thiophene

ge, and a hydroxyl functionalized dicyanomethylendihydrofuran based acceptor. The chromophore was incorporated into a 3D thermosetting polyurethane network through a three hydroxyl group attachment to both ends of the chromophore, in anhydrous dioxane and excess tolylenediisocyanate (TDI).

dynamic alignment stability of the chromophore was enhanced by 25 over that of the single end attached polymer analog. 224967-76-39p

224967-75-3P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (LTR chromophore monomer; a trifunctionalized high  $\mu\beta$  chromophore and 3D polyurethane network with enhanced NLO alignment stability for electrooptical devices) 224967-75-3 CAPLUS Propanedinitrile, 2-[4-[5-[2-[4-[bis[2-[[(1,1-

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-

thienyl]ethenyl]-3-cyano-5-(4-hydroxybutyl)-5-methyl-2(5H)-furanylidene](CA INDEX NAME)

L65 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

$$\begin{array}{c} & & \\$$

L65 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

\_ (CH2) 4 = OH

dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-

thienyl]ethenyl]-3-cyano-5-(4-hydroxybutyl)-5-methyl-2(5H)-furanylidene]-, polymer with 2,4-diisocyanato-1-methylbenzene and 2,2',2'-nitrilotris[ethanol] (921) (CA INDEX NAME)

CM 1

CRN 224967-75-3 CMF C51 H76 N4 O4 S Si2

L65 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-B

\_ (CH<sub>2</sub>)<sub>4</sub>−OH

C-CN

2

CM

102-71-6 C6 H15 N O3

сн<sub>2</sub>-сн<sub>2</sub>-он но-сн2-сн2-и-сн2-сн2-он

L65 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L65 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1999:107637 Document No. 130:259118 Femtosecond, Frequency-Agile, Phase-Sensitive-Detected, Multi-Wave-Mixing Nonlinear Optical

Journal of Physical Chemistry A, 103(14), 229U-23U1 (anglism, 1257).

CODEM: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB Degenerate four-wave mixing (DFWM) spectroscopy is modified to exploit fentosecond pulses, phase-sensitive-detection, frequency (wavelength) agility, two-color (nearly degenerate multi-wave mixing) radiation, and improved signal-to-noise capabilities that can be realized through a combination of new solid state lasers, nonlinear optical components, and novel design concepts. The resulting time-resolved nonlinear optical techniques permit instantaneous optical nonlinearities, such as two-photon absorption cross sections, to be accurately measured over the spectral range from 450 to 2500 mm (and with significantly greater effort from 225 to 5000 mm). The power of the new techniques is illustrated by their application to the definition of Hg two-photon resonances of C60 and C70 as well as to the characterization of optical nonlinearities in two linear chromophores of putative utility for sensor protection and electrooptic modulation. Explicitly, these measurements provide accurate determination of both transition energies and transition moments (matrix elements connecting the

two photon levels). Results are compared to those previously reported in the literature illustrating the advantages and problems associated with particular measurement techniques. All of the mols. studied exhibit two-photon absorption coeffs. comparable to that of GaAs, the most studied

ied
putative sensor protection material (based on use of electronic optical
nonlinearity). Pemtosecond pulse techniques are shown, in all cases, to
be necessary to avoid complications arising from excited-state absorption
and relaxation phenomena. The importance of phase-sensitive detection in
identifying complications from overlapping transitions is illustrated.
213131-88-7

RL: PRP (Properties)

: PKF (Properties) (femtosecond, frequency-agile, phase-sensitive-detected, multi-wave-mixing nonlinear optical spectroscopy applied to  $\pi$ -electron photonic materials)

Propared in Fraction proteins materials, 213131-98-7 CAPLUS Propared initrile, 2-[4-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 1998;550105 Document No. 129;246191 Original Reference No. 129;50125a,50128a High electro-optic coefficient from a polymer containing high μβ chromophores. Wang, Fang; Ren, Albert S.; He, Mingqian; Harper, Aaron W.

Dalton, Larry R.; Garner, Sean M.; Zhang, Hua; Chen, Antao; Steier, William H. (Department of Chemistry, Loker Hydrocarbon Research

William H. (Department or Chemistry, August 2, 1981).
Institute,
University of Southern California, Los Angeles, CA, 90089-1661, USA).
Polymeric Materials Science and Engineering, 78, 42-43 (English)
1998. CODEN: PMSEDG. ISSN: 0743-0515. Publisher: American
Chemical Society.

AB The electrooptical coefficient (r33) values of PMMA doped (16.6%) with a

furan ring-based NLO chromophore (FTC-2 $\lambda$ cO) are reported. FTC-2 $\lambda$ cO has excellent solubility, high thermal stability, a relatively low

excellent solubility, nigh thelmel scauzer, and chromophore absorption maximum, and a very high r33.

12 213131-98-7

RL: MGA (Modifier or additive use); PRP (Properties); USES (Uses) (electrooptical coefficient of NLO chromophore in PMMA)

RN 213131-98-7 CAPLUS

CN Propanedinitrile, 2=[4-[2-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3,4-dibutyl-2-thienyl]ethenyl]-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN 3:532284 Document No. 129:276799 Original Reference No. 129:56435a,56438a

56435a,56438a
Design, synthesis and characterization of a novel substituted dicyanomethylendihydrofuran based high-β NLO chromophore and its polymers with exceptionally high electro-optic coefficients. Wang, Fan-Ren, Albert A.; He, Mingqian; Lee, Michael S.; Harper, Aaron W.; Dalton Larry R.; Zhang, Hua; Garner, Sean M.; Chen, Antao; Steier, William H. (Loker Bydrocarbon Inst. and Dep. Chem., Univ. Southern California, Los Angeles, CA, 90089-1661, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 39(2), 1055-1066 (English) 1998. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemican Chemican Society, Division of Polymer Chemistry). Chemical Society, Division of Polymer Chemistry.

A second order nonlinear optical chromophore having the structure I and exhibiting high mol. nonlinearity, high thermal stability, and low optical

absorption was prepared and characterized. Excellent optical quality films

were obtained when I was co-dissolved in 1,2-dichloroethane with poly(Me methacrylate) (PMMA) and spin-cast onto ITO-coated glass substrates. An electrooptic coefficient of 56.9 pm/V at 1.06  $\mu$ m was achieved with a

loading
d. of 16.6 weight %. The film absorption maximizes at 630 nm and the
propagation optical loss was found to be 0.75 dB/cm using the "immersion
technique". An observed attenuation of the electrooptic coefficient was predicted

icted by the extended London theory when the mol. shape was taken into account. Covalent attachment of I to a crosslinked polyurethane network resulted

a maximum electrooptic coefficient of 42 pm/V at 1.06 um with a loading of 15

weight %. The decrease of the electrooptic coefficient of the polyurethanes

compared to those of the PMMA composites was significant and attributed

the lower poling efficiency of the covalently attached system where the chromophores have less freedom than in the case of doped systems. Bias poled modulators and high-speed electrooptic modulators were fabricated with the patroital attached. poled modulators and high-speed electrooptic modulators were fusing the materials.
213131-98-7D, reaction products with polyurethanes
RL: PRP (Properties)
(design, synthesis and characterization of substituted
dicyanomethylendihydrofuran-based high-β nonlinear optical

1995:752764 Document No. 124:85310 Original Reference No. 124:1805a,1808a Synthesis of substituted dicyanomethylendihydrofurans. Melikian, Gaguik; Rouessac, Francis P.; Alexandre, Christian (Laboratoire de Synthesic Organique, Faculte des Sciences, Le Mans, 72017, Fr.). Synthetic Communications, 25(19), 3045-51 (English) 1995. CODEN: SYNCAV. ISSN: 0039-7911. OTHER SOURCES: CASREACT 124:8531. Publisher: Dekker. ISSN: 0039-7911. OTHER SOURCES: CASREACT 124:8531. Publisher: Dekker. As a simple and efficient method for the preparation of the title compds. is described from α-ketols and malononitrile in the presence of sodium ethylate at room temperature These compds. lead to unsatd. derivs. by condensation with aldehydes. For example, condensation reaction of propanedinitriie and 3-hydroxy-3-methyl-2-butanone gave (3-cyano-2,5-dihydro-4,5,5-trimethyl-2-furanylidene)propanedinitrile.

17 171082-36-3P (Synthetic preparation); PREP (Preparation) (preparation of dicyanomethylendihydrofurans from hydroxy ketones and propanedinitrile).

RN 171082-36-3 (CAPUS)

CN Propanedinitrile, 2-[3-cyano-4-[2-(2-furanyl)ethenyl]-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

L65 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

ANSWER 52 OF 53 CAPUS COPYRIGHT 2010 ACS on STN (Continued) chromophore and chromophore doped and modified polymers with exceptionally high electrooptic coeffs.) 21311-98-7 CAPUS Propanedinitrile, 2-[4-[5-[2-[4-[bis[2-(acetyloxy)ethyl]amino]phenyl]ethenyl]-3, 4-dibutyl-2-thienyl]ethenyl-3-cyano-5,5-dimethyl-2(5H)-furanylidene]- (CA INDEX NAME)

RL: FRF (Properties); SFN (Synthetic preparation); FREF (Preparation) (design, synthesis and characterization of substituted dicyanomethylendihydrofuran-based high- $\beta$  nonlinear optical chromophore and chromophore doped and modified polymers with exceptionally high electrooptic coeffs.

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